Full wwPDB X-ray Structure Validation Report ⓘ

Dec 11, 2024 – 03:17 am GMT

PDB ID	:	8PWV
Title	:	PfRH5 bound to monoclonal antibody MAD8-502
Authors	:	Farrell, B.; Higgins, M.K.
Deposited on	:	2023-07-21
Resolution	:	2.07 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

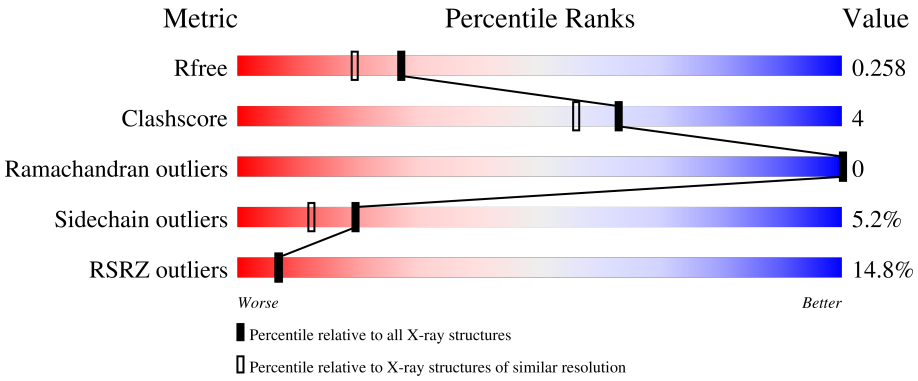
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3436 (2.08-2.04)
Clashscore	180529	3661 (2.08-2.04)
Ramachandran outliers	177936	3649 (2.08-2.04)
Sidechain outliers	177891	3649 (2.08-2.04)
RSRZ outliers	164620	3436 (2.08-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	338	14% 75% 9% • 16%
1	C	338	11% 75% 9% • 16%
1	E	338	17% 70% 12% • 16%
1	G	338	14% 71% 11% • 17%
2	B	252	5% 78% 10% • 10%

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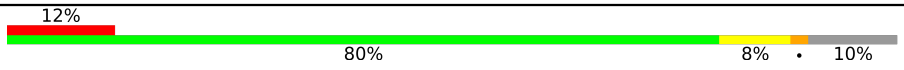
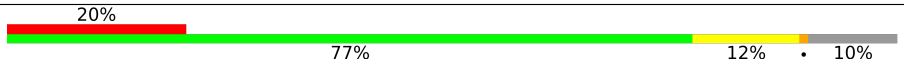
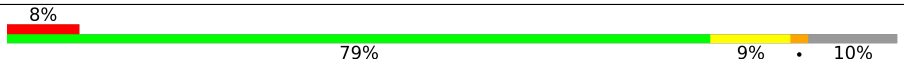
Mol	Chain	Length	Quality of chain
2	D	252	
2	F	252	
2	H	252	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16925 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Reticulocyte-binding protein homolog 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2414	1559	405	437	13			
1	C	284	Total	C	N	O	S	0	0	0
			2414	1559	405	437	13			
1	E	283	Total	C	N	O	S	0	0	0
			2405	1554	403	435	13			
1	G	281	Total	C	N	O	S	0	0	0
			2390	1545	400	432	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	TYR	CYS	engineered mutation	UNP Q8IFM5
A	216	ALA	THR	engineered mutation	UNP Q8IFM5
A	299	ALA	THR	engineered mutation	UNP Q8IFM5
C	203	TYR	CYS	engineered mutation	UNP Q8IFM5
C	216	ALA	THR	engineered mutation	UNP Q8IFM5
C	299	ALA	THR	engineered mutation	UNP Q8IFM5
E	203	TYR	CYS	engineered mutation	UNP Q8IFM5
E	216	ALA	THR	engineered mutation	UNP Q8IFM5
E	299	ALA	THR	engineered mutation	UNP Q8IFM5
G	203	TYR	CYS	engineered mutation	UNP Q8IFM5
G	216	ALA	THR	engineered mutation	UNP Q8IFM5
G	299	ALA	THR	engineered mutation	UNP Q8IFM5

- Molecule 2 is a protein called monoclonal antibody MAD8-502.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1725	1090	288	338	9			
2	D	227	Total	C	N	O	S	0	1	0
			1725	1090	287	339	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	226	Total	C	N	O	S	0	1	0
			1716	1084	285	338	9			
2	H	226	Total	C	N	O	S	0	1	0
			1718	1085	286	338	9			

- Molecule 3 is water.

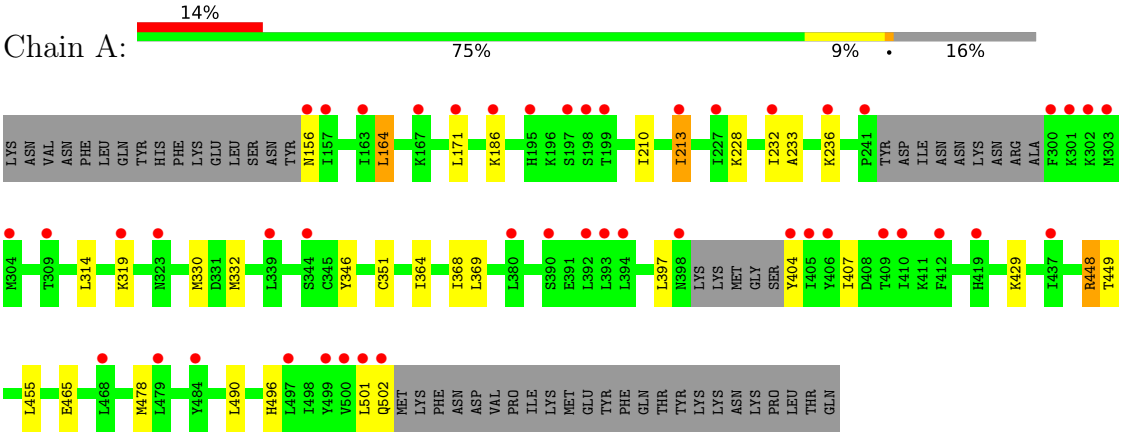
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	43	Total	O	0	0
			43	43		
3	B	92	Total	O	0	0
			92	92		
3	C	69	Total	O	0	0
			69	69		
3	D	37	Total	O	0	0
			37	37		
3	E	102	Total	O	0	0
			102	102		
3	F	30	Total	O	0	0
			30	30		
3	G	10	Total	O	0	0
			10	10		
3	H	35	Total	O	0	0
			35	35		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

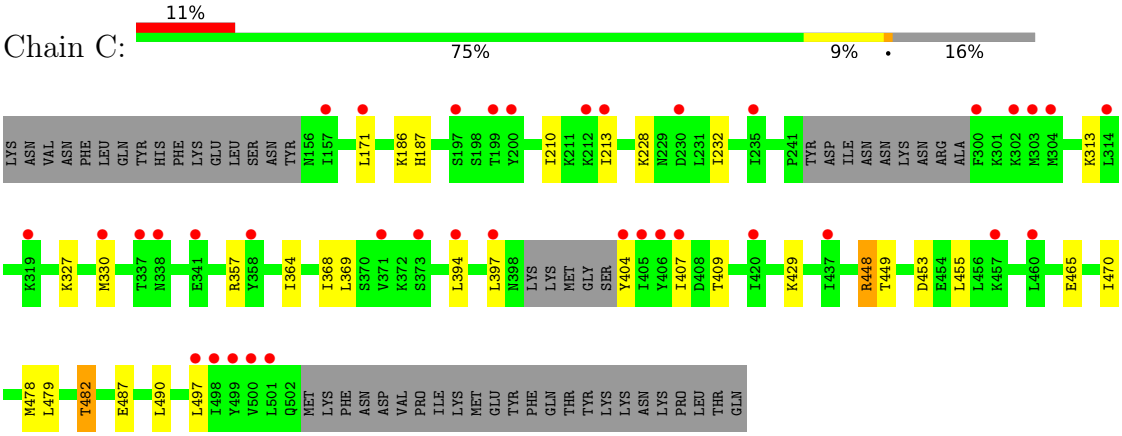
• Molecule 1: Reticulocyte-binding protein homolog 5

Chain A:



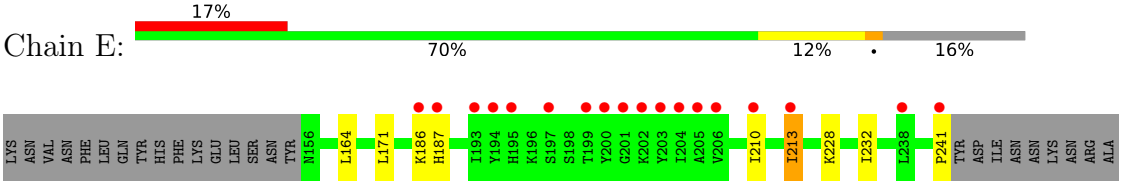
• Molecule 1: Reticulocyte-binding protein homolog 5

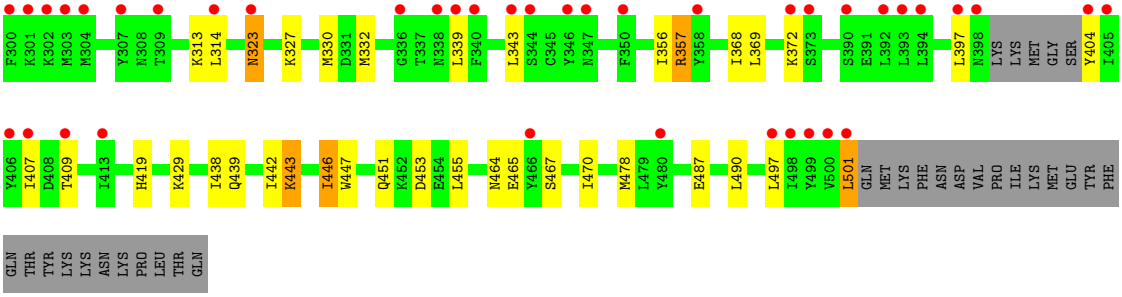
Chain C:



• Molecule 1: Reticulocyte-binding protein homolog 5

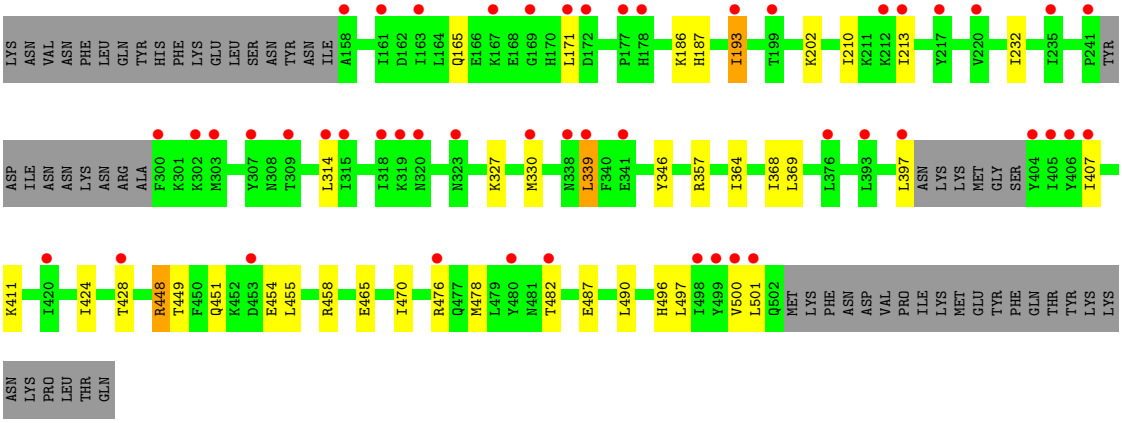
Chain E:





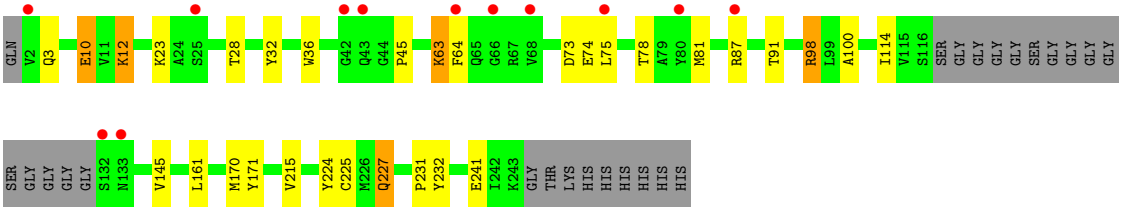
• Molecule 1: Reticulocyte-binding protein homolog 5

Chain G:



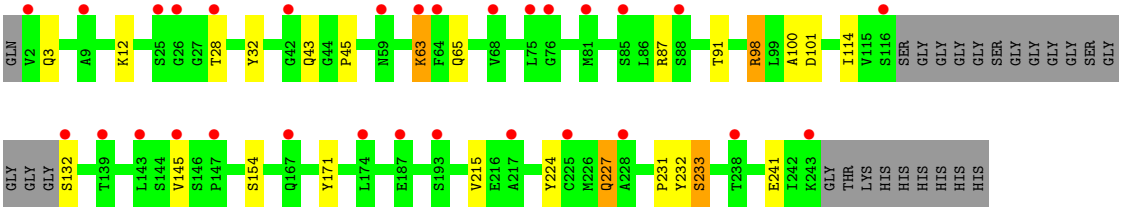
• Molecule 2: monoclonal antibody MAD8-502

Chain B:



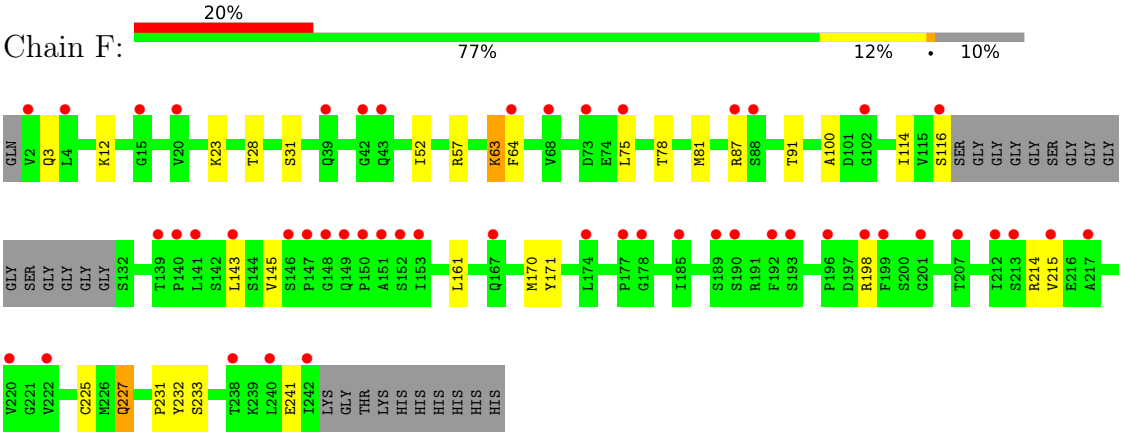
• Molecule 2: monoclonal antibody MAD8-502

Chain D:



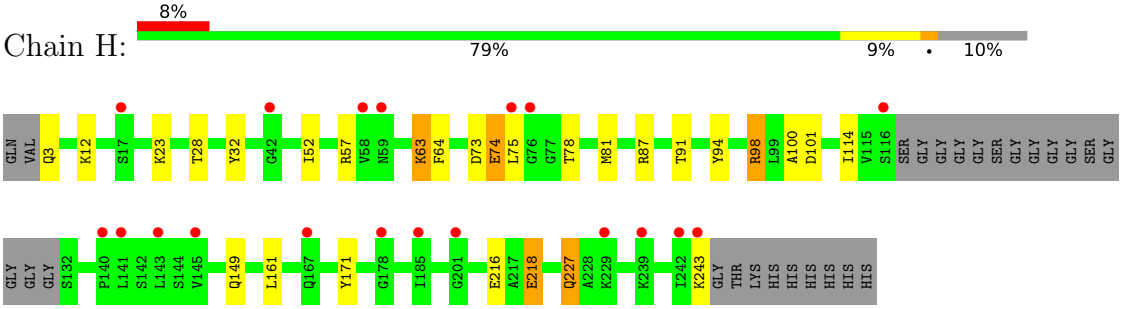
• Molecule 2: monoclonal antibody MAD8-502

Chain F:



• Molecule 2: monoclonal antibody MAD8-502

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.97Å 158.01Å 113.02Å 90.00° 94.59° 90.00°	Depositor
Resolution (Å)	79.00 – 2.07 79.00 – 2.07	Depositor EDS
% Data completeness (in resolution range)	96.2 (79.00-2.07) 96.2 (79.00-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 2.07Å)	Xtriage
Refinement program	BUSTER 2.10.4 (20-OCT-2021)	Depositor
R, R_{free}	0.269 , 0.279 0.250 , 0.258	Depositor DCC
R_{free} test set	15798 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	49.4	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 78.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16925	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.18 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8431e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.39	0/2464	0.54	0/3307
1	C	0.39	0/2464	0.55	0/3307
1	E	0.56	0/2455	0.61	0/3295
1	G	0.37	0/2440	0.55	0/3274
2	B	0.42	0/1763	0.65	0/2388
2	D	0.39	0/1766	0.62	0/2393
2	F	0.38	0/1757	0.60	0/2382
2	H	0.39	0/1759	0.62	0/2383
All	All	0.42	0/16868	0.59	0/22729

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2414	0	2430	15	0
1	C	2414	0	2430	15	0
1	E	2405	0	2422	30	0
1	G	2390	0	2407	20	0
2	B	1725	0	1685	17	0
2	D	1725	0	1681	11	0
2	F	1716	0	1668	15	0
2	H	1718	0	1672	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	43	0	0	0	0
3	B	92	0	0	0	0
3	C	69	0	0	1	0
3	D	37	0	0	0	0
3	E	102	0	0	1	0
3	F	30	0	0	0	0
3	G	10	0	0	0	0
3	H	35	0	0	0	0
All	All	16925	0	16395	128	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (128) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:356:ILE:CD1	1:E:356:ILE:CG1	1.77	1.62
1:E:438:ILE:CD1	1:E:438:ILE:CG1	1.76	1.62
2:D:227:GLN:HE21	2:D:233:SER:HB2	1.26	1.00
2:D:227:GLN:NE2	2:D:233:SER:HB2	1.79	0.96
1:G:478:MET:O	1:G:482:THR:HG23	1.78	0.84
2:H:161:LEU:HD22	2:H:227:GLN:HG3	1.69	0.75
1:E:357:ARG:CG	1:E:446:ILE:HB	2.20	0.72
2:B:10:GLU:HG2	2:B:12:LYS:HD3	1.74	0.69
1:E:357:ARG:HG3	1:E:446:ILE:HB	1.78	0.66
1:E:187:HIS:HE2	1:E:470:ILE:HD12	1.61	0.66
1:C:397:LEU:HD23	1:C:407:ILE:HG13	1.79	0.64
1:G:448:ARG:NH2	1:G:449:THR:O	2.30	0.64
1:G:454:GLU:HG3	1:G:458:ARG:HD2	1.78	0.64
1:A:351:CYS:HB3	1:A:455:LEU:HD22	1.78	0.63
1:C:448:ARG:NH2	1:C:449:THR:O	2.33	0.62
2:H:161:LEU:CD2	2:H:227:GLN:HG3	2.30	0.61
1:A:448:ARG:NH1	1:A:449:THR:O	2.34	0.60
1:A:404:TYR:HB2	1:A:407:ILE:HD13	1.83	0.60
1:E:438:ILE:CD1	1:E:438:ILE:CB	2.76	0.59
1:C:478:MET:O	1:C:482:THR:HG22	2.03	0.58
2:F:161:LEU:HD22	2:F:227:GLN:HG3	1.85	0.58
2:F:145:VAL:HG21	2:F:215:VAL:HG21	1.87	0.57
1:G:186:LYS:HG3	1:G:210:ILE:HD13	1.87	0.57
1:C:186:LYS:HG3	1:C:210:ILE:HD13	1.88	0.56
2:B:161:LEU:HD22	2:B:227:GLN:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:LYS:HG3	1:E:210:ILE:HD13	1.87	0.56
1:E:404:TYR:HB2	1:E:407:ILE:HD13	1.87	0.56
1:A:171:LEU:HD12	1:A:228:LYS:HG3	1.87	0.56
1:A:186:LYS:HG3	1:A:210:ILE:HD13	1.88	0.56
2:F:227:GLN:NE2	2:F:233:SER:OG	2.40	0.55
1:A:369:LEU:HD11	2:B:28:THR:HG21	1.88	0.55
2:B:32:TYR:CD1	2:B:98:ARG:HG3	2.42	0.54
1:G:428:THR:HG22	1:G:476:ARG:HD2	1.89	0.54
1:E:439:GLN:O	1:E:442:ILE:HG22	2.07	0.54
2:B:161:LEU:CD2	2:B:227:GLN:HG3	2.39	0.53
2:F:161:LEU:CD2	2:F:227:GLN:HG3	2.39	0.53
1:E:369:LEU:HA	1:E:372:LYS:NZ	2.23	0.52
2:B:161:LEU:HD22	2:B:227:GLN:CG	2.39	0.52
1:G:357:ARG:NH1	2:H:101:ASP:OD2	2.43	0.52
1:C:357:ARG:NH2	2:D:101:ASP:OD2	2.43	0.52
2:H:161:LEU:HD22	2:H:227:GLN:CG	2.38	0.52
2:D:32:TYR:CD1	2:D:98:ARG:HG3	2.46	0.51
1:C:171:LEU:HD12	1:C:228:LYS:HG3	1.93	0.51
2:B:10:GLU:CG	2:B:12:LYS:HD3	2.40	0.51
2:D:63:LYS:HZ1	2:D:132:SER:N	2.08	0.51
1:A:164:LEU:HG	1:A:478:MET:HB3	1.93	0.50
2:H:52:ILE:HD12	2:H:57:ARG:HD2	1.93	0.50
2:F:52:ILE:HD12	2:F:57:ARG:HD2	1.94	0.50
1:G:369:LEU:HD11	2:H:28:THR:HG21	1.94	0.50
2:H:23:LYS:HG2	2:H:78:THR:HG23	1.94	0.50
2:F:161:LEU:HD22	2:F:227:GLN:CG	2.42	0.49
2:H:74:GLU:HB3	2:H:75:LEU:HD12	1.92	0.49
1:G:165:GLN:H	1:G:482:THR:CG2	2.25	0.49
1:G:424:ILE:O	1:G:428:THR:HG23	2.12	0.49
1:E:241:PRO:HB3	1:E:409:THR:HG21	1.95	0.49
1:C:479:LEU:HA	1:C:482:THR:HG23	1.94	0.49
1:G:193:ILE:HD12	1:G:339:LEU:HG	1.95	0.49
1:E:419:HIS:HD2	3:E:682:HOH:O	1.97	0.48
1:E:369:LEU:HD11	2:F:28:THR:HG21	1.95	0.48
2:H:100:ALA:HB1	2:H:171:TYR:CE2	2.49	0.48
1:C:369:LEU:HD11	2:D:28:THR:HG21	1.96	0.47
2:D:100:ALA:HB1	2:D:171:TYR:CE2	2.49	0.47
2:B:145:VAL:HG21	2:B:215:VAL:HG21	1.96	0.46
1:E:442:ILE:HG23	1:E:443:LYS:HG3	1.97	0.46
2:F:100:ALA:HB1	2:F:171:TYR:CE2	2.50	0.46
1:E:368:ILE:HG22	1:E:372:LYS:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:231:PRO:HA	2:B:232:TYR:HA	1.79	0.46
1:E:497:LEU:O	1:E:501:LEU:HB3	2.15	0.46
1:A:397:LEU:HD23	1:A:407:ILE:HG13	1.98	0.45
2:B:100:ALA:HB1	2:B:171:TYR:CE2	2.51	0.45
2:B:74:GLU:O	2:B:75:LEU:HB2	2.16	0.45
1:E:368:ILE:O	1:E:372:LYS:HG3	2.17	0.45
1:E:446:ILE:HD12	2:F:31:SER:HB2	1.97	0.45
1:E:446:ILE:HG13	1:E:447:TRP:CD1	2.52	0.45
1:G:193:ILE:HG12	1:G:202:LYS:HB2	1.98	0.45
1:E:213:ILE:HG12	1:E:332:MET:HE2	1.99	0.45
2:H:218:GLU:H	2:H:218:GLU:HG3	1.62	0.45
1:A:496:HIS:CE1	1:A:501:LEU:HD13	2.52	0.44
1:G:428:THR:HG22	1:G:476:ARG:CD	2.47	0.44
2:B:45:PRO:HD3	2:B:224:TYR:CE1	2.52	0.44
1:E:171:LEU:HB2	1:E:232:ILE:HG12	2.00	0.44
1:C:364:ILE:HG22	1:C:368:ILE:HD13	2.00	0.44
1:G:397:LEU:HD21	1:G:497:LEU:HD21	2.00	0.44
1:E:397:LEU:HD21	1:E:497:LEU:HD21	2.00	0.44
1:A:346:TYR:HA	1:C:313:LYS:HD3	2.01	0.43
1:C:171:LEU:HB2	1:C:232:ILE:HG12	2.00	0.43
2:H:32:TYR:CD1	2:H:98:ARG:HG3	2.54	0.43
1:G:171:LEU:HB2	1:G:232:ILE:HG12	2.00	0.43
1:E:323:ASN:HD22	1:E:323:ASN:HA	1.69	0.43
1:A:171:LEU:HB2	1:A:232:ILE:HG12	2.01	0.43
1:C:404:TYR:HB3	1:C:407:ILE:HD13	2.01	0.43
2:F:170:MET:CE	2:F:225:CYS:HB2	2.48	0.43
1:A:213:ILE:HG12	1:A:332:MET:HE2	2.00	0.43
2:D:145:VAL:HG21	2:D:215:VAL:HG21	2.01	0.42
2:H:91:THR:HG23	2:H:114:ILE:HA	2.01	0.42
1:E:442:ILE:O	1:E:446:ILE:HG23	2.19	0.42
2:D:231:PRO:HA	2:D:232:TYR:HA	1.80	0.42
2:F:231:PRO:HA	2:F:232:TYR:HA	1.81	0.42
1:E:464:ASN:O	1:E:467:SER:HB2	2.20	0.42
2:H:63:LYS:HD2	2:H:64:PHE:CZ	2.55	0.42
1:E:164:LEU:HG	1:E:478:MET:HB3	2.01	0.42
1:A:156:ASN:OD1	1:A:319:LYS:HE2	2.19	0.42
2:D:91:THR:HG23	2:D:114:ILE:HA	2.02	0.42
1:E:171:LEU:O	1:E:228:LYS:HE2	2.20	0.41
1:E:372:LYS:HB2	1:E:372:LYS:HE2	1.72	0.41
2:B:23:LYS:HG2	2:B:78:THR:HG23	2.01	0.41
2:F:91:THR:HG23	2:F:114:ILE:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:LEU:HD21	1:C:497:LEU:HD21	2.02	0.41
1:C:187:HIS:NE2	1:C:470:ILE:HD12	2.35	0.41
1:E:313:LYS:HD3	1:G:346:TYR:HA	2.02	0.41
2:B:36:TRP:CE2	2:B:81:MET:HB2	2.55	0.41
2:B:91:THR:HG23	2:B:114:ILE:HA	2.02	0.41
2:B:170:MET:CE	2:B:225:CYS:HB2	2.51	0.41
1:G:496:HIS:CD2	1:G:500:VAL:HG21	2.56	0.41
2:B:63:LYS:HD2	2:B:64:PHE:CZ	2.55	0.41
1:G:364:ILE:HG22	1:G:368:ILE:HD13	2.03	0.41
1:E:397:LEU:HD23	1:E:407:ILE:HG13	2.02	0.41
2:F:23:LYS:HG2	2:F:78:THR:HG23	2.02	0.41
2:H:81:MET:HE1	2:H:94:TYR:CD2	2.56	0.41
1:A:364:ILE:HG22	1:A:368:ILE:HD13	2.02	0.40
1:C:357:ARG:HD3	3:C:623:HOH:O	2.20	0.40
2:F:63:LYS:HD2	2:F:64:PHE:CZ	2.56	0.40
1:G:497:LEU:O	1:G:501:LEU:HB3	2.21	0.40
1:A:233:ALA:HA	1:A:236:LYS:HE3	2.03	0.40
2:F:81:MET:HE3	2:F:81:MET:HB3	2.00	0.40
1:G:187:HIS:NE2	1:G:470:ILE:HD12	2.36	0.40
1:G:397:LEU:HD23	1:G:407:ILE:HG13	2.03	0.40
2:D:45:PRO:HD3	2:D:224:TYR:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	278/338 (82%)	274 (99%)	4 (1%)	0	100	100
1	C	278/338 (82%)	275 (99%)	3 (1%)	0	100	100
1	E	277/338 (82%)	269 (97%)	8 (3%)	0	100	100
1	G	275/338 (81%)	271 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	223/252 (88%)	217 (97%)	6 (3%)	0	100	100
2	D	224/252 (89%)	219 (98%)	5 (2%)	0	100	100
2	F	223/252 (88%)	215 (96%)	8 (4%)	0	100	100
2	H	223/252 (88%)	218 (98%)	5 (2%)	0	100	100
All	All	2001/2360 (85%)	1958 (98%)	43 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	275/327 (84%)	266 (97%)	9 (3%)	33	27
1	C	275/327 (84%)	262 (95%)	13 (5%)	22	15
1	E	274/327 (84%)	256 (93%)	18 (7%)	14	7
1	G	272/327 (83%)	259 (95%)	13 (5%)	21	15
2	B	189/202 (94%)	180 (95%)	9 (5%)	21	15
2	D	189/202 (94%)	178 (94%)	11 (6%)	17	9
2	F	188/202 (93%)	177 (94%)	11 (6%)	16	9
2	H	188/202 (93%)	176 (94%)	12 (6%)	14	8
All	All	1850/2116 (87%)	1754 (95%)	96 (5%)	19	12

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	LEU
1	A	213	ILE
1	A	314	LEU
1	A	330	MET
1	A	429	LYS
1	A	448	ARG

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Mol	Chain	Res	Type
1	A	465	GLU
1	A	490	LEU
1	A	502	GLN
2	B	3	GLN
2	B	10	GLU
2	B	12	LYS
2	B	63	LYS
2	B	73	ASP
2	B	87	ARG
2	B	98	ARG
2	B	227	GLN
2	B	241	GLU
1	C	213	ILE
1	C	327	LYS
1	C	330	MET
1	C	394	LEU
1	C	409	THR
1	C	429	LYS
1	C	448	ARG
1	C	453	ASP
1	C	455	LEU
1	C	465	GLU
1	C	482	THR
1	C	487	GLU
1	C	490	LEU
2	D	3	GLN
2	D	12	LYS
2	D	43	GLN
2	D	63	LYS
2	D	65	GLN
2	D	87	ARG
2	D	98	ARG
2	D	154	SER
2	D	227	GLN
2	D	233	SER
2	D	241	GLU
1	E	213	ILE
1	E	314	LEU
1	E	323	ASN
1	E	327	LYS
1	E	330	MET
1	E	339	LEU

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Mol	Chain	Res	Type
1	E	343	LEU
1	E	357	ARG
1	E	429	LYS
1	E	443	LYS
1	E	446	ILE
1	E	451	GLN
1	E	453	ASP
1	E	455	LEU
1	E	465	GLU
1	E	487	GLU
1	E	490	LEU
1	E	501	LEU
2	F	3	GLN
2	F	12	LYS
2	F	63	LYS
2	F	75	LEU
2	F	87	ARG
2	F	116	SER
2	F	143	LEU
2	F	198	ARG
2	F	214	ARG
2	F	227	GLN
2	F	241	GLU
1	G	193	ILE
1	G	213	ILE
1	G	314	LEU
1	G	327	LYS
1	G	330	MET
1	G	339	LEU
1	G	411	LYS
1	G	448	ARG
1	G	451	GLN
1	G	455	LEU
1	G	465	GLU
1	G	487	GLU
1	G	490	LEU
2	H	3	GLN
2	H	12	LYS
2	H	63	LYS
2	H	73	ASP
2	H	74	GLU
2	H	87	ARG

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Mol	Chain	Res	Type
2	H	98	ARG
2	H	149	GLN
2	H	216	GLU
2	H	218	GLU
2	H	227	GLN
2	H	243	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	284/338 (84%)	1.19	47 (16%) 5 5	55, 74, 97, 112	0
1	C	284/338 (84%)	1.03	37 (13%) 9 9	55, 67, 89, 102	0
1	E	283/338 (83%)	1.38	58 (20%) 3 3	33, 67, 98, 113	0
1	G	281/338 (83%)	1.26	49 (17%) 5 4	61, 81, 104, 117	0
2	B	227/252 (90%)	0.76	12 (5%) 33 34	50, 59, 75, 90	0
2	D	227/252 (90%)	1.03	30 (13%) 8 9	48, 70, 88, 101	1 (0%)
2	F	226/252 (89%)	1.36	50 (22%) 3 2	53, 74, 119, 155	1 (0%)
2	H	226/252 (89%)	0.94	19 (8%) 18 20	52, 66, 91, 106	1 (0%)
All	All	2038/2360 (86%)	1.13	302 (14%) 7 7	33, 70, 99, 155	3 (0%)

All (302) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	75	LEU	7.5
1	E	501	LEU	6.4
1	G	500	VAL	6.1
1	G	404	TYR	5.7
2	D	75	LEU	5.6
1	E	499	TYR	5.4
1	G	235	ILE	5.4
2	B	75	LEU	5.3
1	E	498	ILE	5.2
1	E	404	TYR	5.2
1	C	499	TYR	5.2
1	E	500	VAL	5.1
1	A	404	TYR	4.8
1	A	499	TYR	4.8
2	F	242	ILE	4.8
1	E	200	TYR	4.8

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Mol	Chain	Res	Type	RSRZ
1	E	203	TYR	4.7
1	A	302	LYS	4.6
1	C	500	VAL	4.5
1	E	405	ILE	4.4
2	H	243	LYS	4.3
1	C	404	TYR	4.3
2	F	217	ALA	4.2
1	A	405	ILE	4.1
2	F	147	PRO	4.1
1	A	500	VAL	4.0
1	A	241	PRO	4.0
1	C	300	PHE	4.0
1	E	497	LEU	4.0
2	H	75	LEU	3.9
1	E	406	TYR	3.9
1	G	300	PHE	3.9
1	C	405	ILE	3.8
1	G	397	LEU	3.8
1	G	338	ASN	3.8
1	G	499	TYR	3.8
1	A	157	ILE	3.8
2	F	212	ILE	3.8
1	A	300	PHE	3.8
1	G	405	ILE	3.8
2	D	63	LYS	3.7
2	F	2	VAL	3.7
2	F	150	PRO	3.7
2	F	215	VAL	3.6
1	G	193	ILE	3.6
2	F	73	ASP	3.6
1	C	373	SER	3.6
2	H	242	ILE	3.5
2	F	88	SER	3.5
1	E	199	THR	3.5
1	G	309	THR	3.5
1	E	336	GLY	3.5
2	F	141	LEU	3.5
1	E	300	PHE	3.4
2	D	2	VAL	3.4
2	H	116	SER	3.4
2	B	2	VAL	3.4
1	G	393	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	F	116	SER	3.3
2	B	42	GLY	3.3
2	H	141	LEU	3.3
2	H	76	GLY	3.2
1	E	323	ASN	3.2
1	A	406	TYR	3.2
1	G	501	LEU	3.2
1	E	303	MET	3.2
1	E	409	THR	3.2
1	G	163	ILE	3.2
2	F	167	GLN	3.1
1	G	302	LYS	3.1
2	D	217	ALA	3.1
1	E	344	SER	3.1
1	C	437	ILE	3.1
1	G	498	ILE	3.1
1	E	390	SER	3.1
2	F	42	GLY	3.0
1	E	346	TYR	3.0
1	E	407	ILE	3.0
1	E	197	SER	3.0
1	G	428	THR	3.0
2	F	148	GLY	3.0
1	E	350	PHE	3.0
1	E	393	LEU	3.0
2	F	143	LEU	3.0
1	C	157	ILE	3.0
1	A	199	THR	3.0
2	D	243	LYS	3.0
1	A	303	MET	3.0
1	G	177	PRO	3.0
2	F	213	SER	2.9
1	C	338	ASN	2.9
2	F	201	GLY	2.9
1	E	394	LEU	2.9
1	A	232	ILE	2.9
1	E	373	SER	2.9
1	E	186	LYS	2.9
1	G	341	GLU	2.9
1	C	200	TYR	2.9
1	E	392	LEU	2.9
1	G	213	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	194	TYR	2.9
1	C	303	MET	2.8
1	C	235	ILE	2.8
1	C	497	LEU	2.8
1	E	238	LEU	2.8
1	E	206	VAL	2.8
2	F	64	PHE	2.8
1	C	498	ILE	2.8
1	G	406	TYR	2.8
1	C	397	LEU	2.8
2	D	116	SER	2.8
1	G	315	ILE	2.7
1	A	393	LEU	2.7
1	A	319	LYS	2.7
2	F	174	LEU	2.7
1	A	398	ASN	2.7
1	G	320	ASN	2.7
2	D	238	THR	2.7
1	G	167	LYS	2.7
1	G	319	LYS	2.7
1	G	172	ASP	2.7
2	F	190	SER	2.6
2	F	220	VAL	2.6
1	C	337	THR	2.6
1	A	156	ASN	2.6
1	E	338	ASN	2.6
1	A	394	LEU	2.6
1	E	187	HIS	2.6
2	H	42	GLY	2.6
2	B	132	SER	2.6
2	F	152[A]	SER	2.6
1	E	343	LEU	2.6
1	E	201	GLY	2.6
1	C	406	TYR	2.6
1	A	163	ILE	2.6
1	G	407	ILE	2.6
2	B	87	ARG	2.6
1	A	197	SER	2.6
2	D	132	SER	2.6
1	A	301	LYS	2.5
1	G	158	ALA	2.5
2	H	58	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	482	THR	2.5
2	F	238	THR	2.5
1	E	241	PRO	2.5
1	E	397	LEU	2.5
1	A	323	ASN	2.5
2	H	167	GLN	2.5
1	A	437	ILE	2.5
2	F	189	SER	2.5
1	A	171	LEU	2.5
2	D	145	VAL	2.5
1	E	340	PHE	2.5
2	D	85	SER	2.5
1	C	302	LYS	2.5
1	C	457	LYS	2.5
2	H	229	LYS	2.5
1	A	339	LEU	2.5
1	G	330	MET	2.5
2	D	228	ALA	2.5
2	F	151	ALA	2.5
2	D	167	GLN	2.5
1	E	358	TYR	2.4
1	G	480	TYR	2.4
1	E	302	LYS	2.4
1	C	407	ILE	2.4
2	H	201	GLY	2.4
1	C	304	MET	2.4
1	A	380	LEU	2.4
1	C	314	LEU	2.4
1	C	501	LEU	2.4
1	E	314	LEU	2.4
2	F	198	ARG	2.4
1	A	309	THR	2.4
2	D	88	SER	2.4
2	F	146	SER	2.4
1	A	213	ILE	2.4
2	B	66	GLY	2.4
2	D	26	GLY	2.4
2	F	240	LEU	2.4
2	D	225	CYS	2.4
1	A	409	THR	2.4
2	F	207	THR	2.4
1	G	241	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	344	SER	2.4
1	E	204	ILE	2.4
1	G	303	MET	2.4
2	H	143	LEU	2.3
1	C	330	MET	2.3
1	A	412	PHE	2.3
1	A	484	TYR	2.3
1	A	227	ILE	2.3
2	F	4	LEU	2.3
2	F	20	VAL	2.3
2	F	199	PHE	2.3
1	A	501	LEU	2.3
1	G	171	LEU	2.3
1	A	304	MET	2.3
2	D	28	THR	2.3
2	D	139	THR	2.3
2	F	140	PRO	2.3
1	C	230	ASP	2.3
2	D	187	GLU	2.3
2	D	174	LEU	2.3
1	C	199	THR	2.3
1	A	236	LYS	2.2
1	A	195	HIS	2.2
2	H	59	ASN	2.2
1	A	392	LEU	2.2
1	E	339	LEU	2.2
1	E	466	TYR	2.2
1	G	217	TYR	2.2
1	G	199	THR	2.2
2	H	17	SER	2.2
1	E	372	LYS	2.2
2	D	59	ASN	2.2
1	A	502	GLN	2.2
1	G	420	ILE	2.2
2	F	43	GLN	2.2
2	F	185	ILE	2.2
2	H	185	ILE	2.2
1	G	376	LEU	2.2
1	E	307	TYR	2.2
2	B	64	PHE	2.2
2	F	192	PHE	2.2
1	C	213	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	420	ILE	2.2
1	E	193	ILE	2.2
1	G	161	ILE	2.2
1	C	171	LEU	2.2
1	C	197	SER	2.2
2	D	25	SER	2.2
2	H	140	PRO	2.2
1	G	169	GLY	2.2
2	F	87	ARG	2.2
2	H	178	GLY	2.2
1	G	178	HIS	2.2
2	H	145	VAL	2.2
1	A	497	LEU	2.1
2	B	25	SER	2.1
2	H	239	LYS	2.1
2	D	147	PRO	2.1
1	E	195	HIS	2.1
2	D	76	GLY	2.1
2	F	15	GLY	2.1
1	G	220	VAL	2.1
2	F	68	VAL	2.1
1	A	410	ILE	2.1
1	A	468	LEU	2.1
1	C	212	LYS	2.1
1	E	213	ILE	2.1
2	D	143	LEU	2.1
1	A	390	SER	2.1
2	D	9	ALA	2.1
1	E	480	TYR	2.1
1	G	307	TYR	2.1
2	B	80	TYR	2.1
1	E	304	MET	2.1
2	B	43	GLN	2.1
2	D	68	VAL	2.1
1	A	186	LYS	2.1
1	C	394	LEU	2.1
1	G	339	LEU	2.1
2	D	64	PHE	2.1
2	D	193	SER	2.1
2	F	153	ILE	2.1
2	F	193	SER	2.1
2	D	42	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	177	PRO	2.1
2	F	178	GLY	2.1
1	C	358	TYR	2.1
1	E	347	ASN	2.1
2	F	149	GLN	2.1
2	B	68	VAL	2.1
1	A	419	HIS	2.1
1	G	314	LEU	2.1
1	E	309	THR	2.1
2	D	81	MET	2.1
1	E	205	ALA	2.0
1	C	341	GLU	2.0
1	E	398	ASN	2.0
2	F	196	PRO	2.0
1	C	319	LYS	2.0
1	E	202	LYS	2.0
1	E	301	LYS	2.0
1	G	476	ARG	2.0
1	A	198	SER	2.0
1	A	479	LEU	2.0
1	C	460	LEU	2.0
2	F	39	GLN	2.0
2	F	139	THR	2.0
1	E	210	ILE	2.0
1	E	413	ILE	2.0
1	G	318	ILE	2.0
1	G	323	ASN	2.0
2	B	133	ASN	2.0
2	F	102	GLY	2.0
1	A	167	LYS	2.0
1	G	212	LYS	2.0
1	C	371	VAL	2.0
2	F	222	VAL	2.0
1	G	453	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.