Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 08:09 PM EDT

PDB ID	:	1G1U
Title	:	THE 2.5 ANGSTROM RESOLUTION CRYSTAL STRUCTURE OF THE RXRALPHA LIGAND BINDING DOMAIN IN TETRAMER IN THE ABSENCE OF LIGAND
Authors	:	Gampe Jr., R.T.; Montana, V.G.; Lambert, M.H.; Wisely, G.B.; Milburn, M.V.; Xu, H.E.
Deposited on	:	2000-10-13
Resolution	:	2.50 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 (i) 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 (1)) were used in the production of this report:

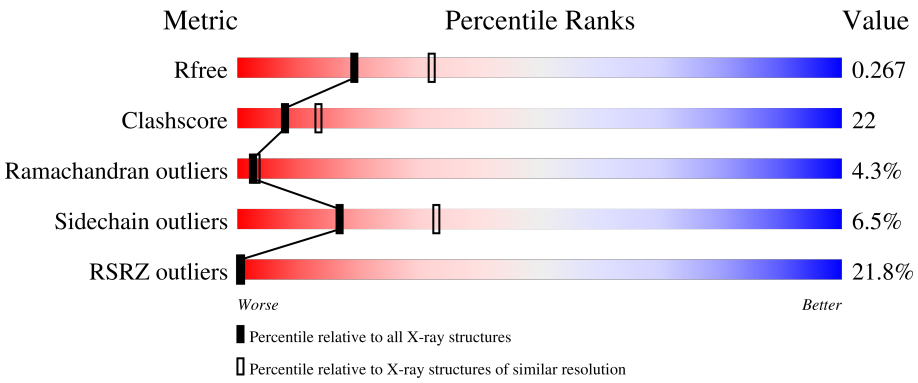
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	238	24% 65% 25% 5% • •
1	B	238	15% 59% 31% 6% •
1	C	238	22% 54% 37% • • 5%
1	D	238	22% 58% 33% 5% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7208 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 RETINOIC ACID RECEPTOR RXR-ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	228	1724	1104	301	310	9	0	0	0
1	B	229	1739	1115	303	312	9	0	0	0
1	C	226	1704	1093	293	309	9	0	0	0
1	D	229	1731	1110	301	311	9	0	0	0

- Molecule 2 is water.

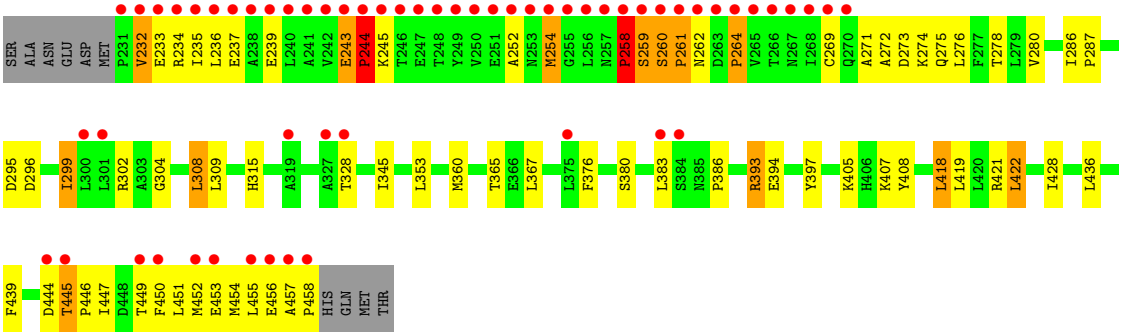
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	85	85	85	0	0
2	B	98	98	98	0	0
2	C	59	59	59	0	0
2	D	68	68	68	0	0

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.

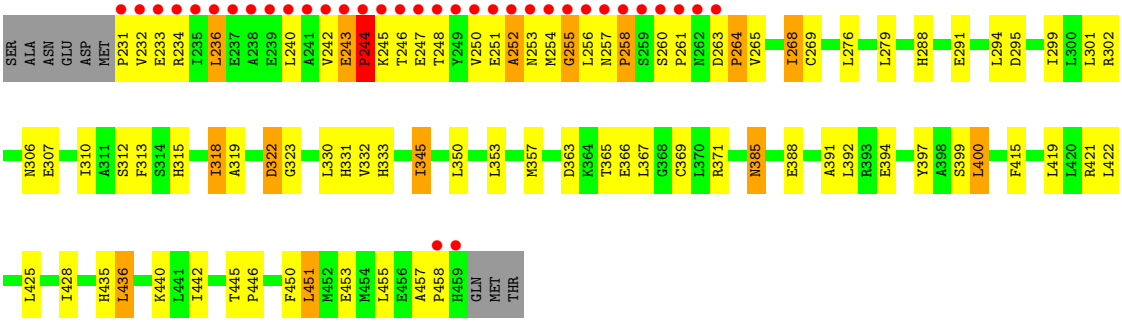
• Molecule 1: RETINOIC ACID RECEPTOR RXR-ALPHA

Chain A:



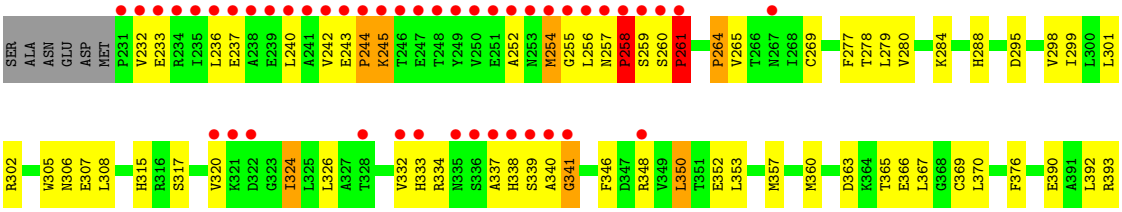
• Molecule 1: RETINOIC ACID RECEPTOR RXR-ALPHA

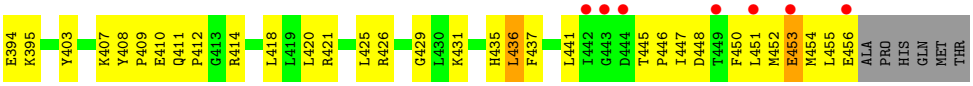
Chain B:



• Molecule 1: RETINOIC ACID RECEPTOR RXR-ALPHA

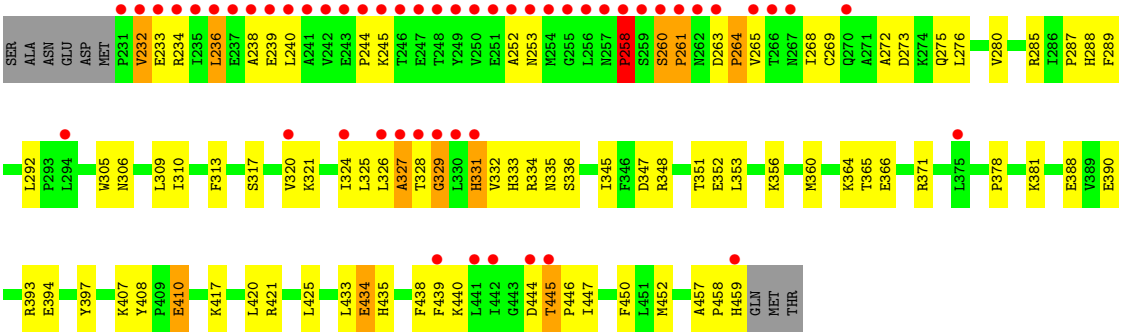
Chain C:





- Molecule 1: RETINOIC ACID RECEPTOR RXR-ALPHA

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.06Å 99.31Å 94.98Å 90.00° 97.38° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.47 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.3 (20.00-2.50) 98.3 (19.47-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.50Å)	Xtriage
Refinement program	CNX 2000	Depositor
R, R_{free}	0.220 , 0.271 0.219 , 0.267	Depositor DCC
R_{free} test set	3201 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å^2)	28.6	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 67.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7208	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

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	0.36	0/1756	0.67	5/2378 (0.2%)
1	B	0.36	0/1773	0.63	3/2403 (0.1%)
1	C	0.35	0/1736	0.60	3/2356 (0.1%)
1	D	0.34	0/1765	0.63	4/2394 (0.2%)
All	All	0.35	0/7030	0.63	15/9531 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	331	HIS	N-CA-C	6.05	127.34	111.00
1	B	258	PRO	N-CA-CB	5.90	110.38	103.30
1	B	244	PRO	N-CA-CB	5.83	110.30	103.30
1	C	258	PRO	N-CA-CB	5.82	110.28	103.30
1	D	244	PRO	N-CA-CB	5.67	110.11	103.30
1	D	258	PRO	N-CA-CB	5.63	110.05	103.30
1	D	261	PRO	N-CA-CB	5.59	110.01	103.30
1	A	258	PRO	N-CA-CB	5.58	110.00	103.30
1	A	264	PRO	N-CA-CB	5.52	109.93	103.30
1	C	244	PRO	N-CA-CB	5.49	109.88	103.30
1	A	458	PRO	N-CA-CB	5.48	109.88	103.30
1	A	261	PRO	N-CA-CB	5.48	109.87	103.30
1	A	244	PRO	N-CA-CB	5.47	109.87	103.30
1	B	261	PRO	N-CA-CB	5.28	109.63	103.30
1	C	261	PRO	N-CA-CB	5.07	109.38	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1724	0	1692	80	0
1	B	1739	0	1719	71	0
1	C	1704	0	1672	92	0
1	D	1731	0	1702	70	0
2	A	85	0	0	1	0
2	B	98	0	0	1	0
2	C	59	0	0	1	0
2	D	68	0	0	2	0
All	All	7208	0	6785	293	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 22.

All (293) 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:C:411:GLN:NE2	1:C:414:ARG:HD2	1.60	1.17
1:C:324:ILE:HD11	1:C:441:LEU:HD21	1.50	0.92
1:C:411:GLN:HE22	1:C:414:ARG:HD2	1.22	0.92
1:A:232:VAL:HG23	1:A:235:ILE:HD12	1.53	0.88
1:D:327:ALA:H	1:D:331:HIS:CE1	1.91	0.87
1:A:233:GLU:HA	1:A:236:LEU:HB3	1.56	0.86
1:C:348:ARG:HD2	1:C:352:GLU:OE2	1.77	0.84
1:A:299:ILE:HD11	1:A:380:SER:HB3	1.59	0.83
1:D:327:ALA:N	1:D:331:HIS:NE2	2.29	0.80
1:A:269:CYS:HG	1:C:269:CYS:HG	1.17	0.79
1:A:235:ILE:HD11	1:A:287:PRO:HD2	1.66	0.77
1:A:232:VAL:O	1:A:236:LEU:N	2.19	0.75
1:B:269:CYS:HG	1:D:269:CYS:HG	0.79	0.74
1:D:263:ASP:O	1:D:265:VAL:N	2.21	0.73
1:A:273:ASP:CG	1:C:265:VAL:HG22	2.11	0.71
1:D:328:THR:N	1:D:331:HIS:NE2	2.38	0.71
1:A:446:PRO:O	1:A:449:THR:HG22	1.90	0.71
1:A:449:THR:HG23	1:A:450:PHE:N	2.07	0.70
1:C:307:GLU:HG2	1:C:425:LEU:HG	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ASP:OD2	1:C:265:VAL:HG22	1.91	0.70
1:D:435:HIS:O	1:D:440:LYS:HE2	1.92	0.70
1:A:444:ASP:HB2	1:C:302:ARG:HH12	1.57	0.69
1:D:232:VAL:HG12	1:D:233:GLU:OE2	1.93	0.69
1:B:445:THR:HB	1:B:446:PRO:HD3	1.73	0.69
1:C:280:VAL:O	1:C:284:LYS:HG3	1.93	0.68
1:C:332:VAL:HG22	1:C:337:ALA:HB2	1.74	0.68
1:D:325:LEU:O	1:D:326:LEU:HD23	1.93	0.67
1:A:447:ILE:O	1:A:451:LEU:HB2	1.94	0.67
1:A:295:ASP:O	1:A:299:ILE:HG22	1.94	0.67
1:B:254:MET:O	1:B:256:LEU:N	2.28	0.67
1:A:235:ILE:O	1:A:239:GLU:HG3	1.95	0.66
1:C:243:GLU:O	1:C:245:LYS:N	2.28	0.66
1:A:302:ARG:NH1	1:C:448:ASP:OD1	2.27	0.66
1:B:302:ARG:HH12	1:D:444:ASP:HB2	1.60	0.66
1:B:310:ILE:HG23	1:B:425:LEU:HD11	1.78	0.66
1:D:310:ILE:HA	1:D:313:PHE:CE2	2.31	0.66
1:C:411:GLN:HE21	1:C:414:ARG:HD2	1.55	0.66
1:C:451:LEU:O	1:C:455:LEU:HD23	1.95	0.65
1:B:254:MET:O	1:B:257:ASN:N	2.29	0.65
1:A:280:VAL:HG11	1:C:454:MET:HB3	1.78	0.64
1:A:274:LYS:O	1:A:278:THR:HG23	1.97	0.64
1:A:233:GLU:O	1:A:237:GLU:HB2	1.98	0.64
1:A:449:THR:HG23	1:A:450:PHE:H	1.60	0.64
1:C:445:THR:HB	1:C:446:PRO:HD3	1.80	0.64
1:D:252:ALA:O	1:D:328:THR:HG23	1.98	0.63
1:C:259:SER:C	1:C:261:PRO:N	2.52	0.63
1:A:235:ILE:HG12	1:A:286:ILE:HD13	1.80	0.63
1:D:268:ILE:HD12	1:D:268:ILE:H	1.64	0.62
1:D:351:THR:HG22	1:D:352:GLU:HG3	1.81	0.62
1:A:450:PHE:O	1:A:454:MET:HG3	2.00	0.62
1:C:411:GLN:NE2	1:C:414:ARG:CD	2.52	0.61
1:B:457:ALA:HB1	1:B:458:PRO:HD2	1.83	0.61
1:B:295:ASP:O	1:B:299:ILE:HG12	2.01	0.61
1:B:248:THR:C	1:B:250:VAL:H	2.04	0.61
1:B:323:GLY:H	1:B:331:HIS:HE1	1.48	0.61
1:D:239:GLU:OE2	1:D:371:ARG:HD3	2.01	0.61
1:D:390:GLU:O	1:D:394:GLU:HG3	2.00	0.60
1:B:345:ILE:HD13	1:B:345:ILE:O	2.01	0.60
1:C:353:LEU:O	1:C:357:MET:HG3	2.01	0.60
1:C:346:PHE:O	1:C:350:LEU:HD22	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:GLU:O	1:C:237:GLU:HG3	2.01	0.59
1:C:288:HIS:CE1	1:C:395:LYS:NZ	2.70	0.59
1:A:299:ILE:CD1	1:A:380:SER:HB3	2.32	0.59
1:A:271:ALA:O	1:A:273:ASP:N	2.35	0.59
1:A:273:ASP:OD1	1:C:264:PRO:HG2	2.03	0.59
1:D:333:HIS:HB2	1:D:335:ASN:OD1	2.03	0.59
1:A:232:VAL:CG2	1:A:235:ILE:HD12	2.27	0.59
1:C:243:GLU:C	1:C:245:LYS:H	2.04	0.59
1:C:376:PHE:CE1	1:C:392:LEU:HD23	2.38	0.58
1:C:288:HIS:CE1	1:C:395:LYS:HZ1	2.21	0.58
1:D:334:ARG:HG2	1:D:334:ARG:HH11	1.67	0.58
1:A:376:PHE:O	1:A:393:ARG:HD3	2.03	0.58
1:C:252:ALA:C	1:C:254:MET:H	2.08	0.58
1:C:435:HIS:C	1:C:436:LEU:HD12	2.24	0.57
1:C:232:VAL:HG23	1:C:369:CYS:SG	2.43	0.57
1:A:232:VAL:O	1:A:232:VAL:HG13	2.04	0.57
1:A:296:ASP:HA	1:A:299:ILE:CG2	2.33	0.57
1:B:315:HIS:O	1:B:318:ILE:HD12	2.03	0.57
1:D:305:TRP:O	1:D:309:LEU:HD23	2.05	0.57
1:B:391:ALA:O	1:B:394:GLU:HG3	2.06	0.56
1:B:345:ILE:HD11	1:B:428:ILE:HG23	1.88	0.56
1:C:279:LEU:HD21	1:C:305:TRP:HA	1.88	0.56
1:D:407:LYS:HG2	1:D:408:TYR:CE1	2.40	0.56
1:B:369:CYS:CB	1:B:400:LEU:HG	2.35	0.55
1:C:255:GLY:C	1:C:257:ASN:H	2.09	0.55
1:C:393:ARG:HD3	1:D:420:LEU:HD13	1.88	0.55
1:D:253:ASN:HA	1:D:329:GLY:N	2.21	0.55
1:D:328:THR:N	1:D:331:HIS:CE1	2.75	0.55
1:D:332:VAL:HG13	1:D:336:SER:HB2	1.89	0.55
1:A:445:THR:OG1	1:A:446:PRO:HD3	2.06	0.55
1:D:234:ARG:HE	1:D:287:PRO:HG3	1.71	0.54
1:A:383:LEU:HD11	1:A:386:PRO:HG3	1.89	0.54
1:D:234:ARG:NE	1:D:287:PRO:HG3	2.22	0.54
1:A:252:ALA:HB3	1:A:328:THR:O	2.07	0.54
1:C:324:ILE:HG23	1:C:346:PHE:CZ	2.43	0.54
1:B:310:ILE:HA	1:B:313:PHE:CE2	2.43	0.54
1:D:240:LEU:HD21	1:D:364:LYS:HD2	1.89	0.54
1:B:315:HIS:O	1:B:318:ILE:HG23	2.07	0.54
1:B:236:LEU:O	1:B:240:LEU:HG	2.08	0.53
1:C:306:ASN:HD21	1:C:429:GLY:C	2.12	0.53
1:D:458:PRO:O	1:D:459:HIS:C	2.46	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:THR:N	1:D:446:PRO:CD	2.72	0.53
1:C:324:ILE:HG12	1:C:332:VAL:CG1	2.38	0.53
1:D:275:GLN:HG3	1:D:309:LEU:HD11	1.90	0.53
1:C:298:VAL:O	1:C:302:ARG:HG3	2.09	0.53
1:D:238:ALA:HA	1:D:285:ARG:HE	1.73	0.53
1:A:436:LEU:N	1:A:436:LEU:HD22	2.24	0.52
1:A:271:ALA:O	1:A:272:ALA:HB3	2.08	0.52
1:C:360:MET:HE1	1:C:418:LEU:HD12	1.91	0.52
1:D:348:ARG:HD3	1:D:352:GLU:OE2	2.09	0.52
1:B:231:PRO:N	1:B:234:ARG:HD3	2.25	0.52
1:A:394:GLU:HG3	1:A:397:TYR:CZ	2.45	0.52
1:B:385:ASN:O	1:B:388:GLU:HG2	2.10	0.52
1:D:356:LYS:O	1:D:360:MET:HG2	2.09	0.52
1:C:348:ARG:HH21	1:C:431:LYS:HD3	1.75	0.52
1:B:232:VAL:HG23	1:B:399:SER:HB3	1.92	0.52
1:A:269:CYS:O	1:A:271:ALA:O	2.28	0.51
1:B:231:PRO:CD	1:B:234:ARG:HH11	2.22	0.51
1:C:363:ASP:OD1	1:C:366:GLU:HG3	2.09	0.51
1:A:243:GLU:O	1:A:244:PRO:C	2.47	0.51
1:B:245:LYS:O	1:B:247:GLU:N	2.43	0.51
1:A:232:VAL:HG22	1:A:235:ILE:HB	1.93	0.51
1:A:233:GLU:O	1:A:237:GLU:CB	2.58	0.51
1:B:268:ILE:HG12	1:B:442:ILE:CD1	2.41	0.51
1:B:330:LEU:HD13	1:B:331:HIS:N	2.26	0.51
1:C:437:PHE:O	1:C:441:LEU:HB2	2.09	0.51
1:C:436:LEU:HD12	1:C:436:LEU:N	2.26	0.51
1:C:411:GLN:HE22	1:C:414:ARG:CD	2.07	0.51
1:A:449:THR:CG2	1:A:450:PHE:N	2.73	0.51
1:C:403:TYR:CZ	1:C:407:LYS:HD3	2.45	0.51
1:C:407:LYS:C	1:C:409:PRO:HD3	2.32	0.51
1:C:411:GLN:HE22	1:C:414:ARG:HH11	1.60	0.50
1:B:232:VAL:HG13	1:B:365:THR:HG23	1.93	0.50
1:B:269:CYS:CB	1:D:269:CYS:HG	2.23	0.50
1:B:367:LEU:O	1:B:371:ARG:HG3	2.12	0.50
1:C:257:ASN:O	1:C:259:SER:N	2.44	0.50
1:D:347:ASP:O	1:D:351:THR:HB	2.12	0.50
1:A:446:PRO:C	1:A:449:THR:HG22	2.30	0.50
1:B:276:LEU:O	1:B:279:LEU:HB3	2.10	0.50
1:D:268:ILE:HD12	1:D:268:ILE:N	2.27	0.50
1:B:369:CYS:HB3	1:B:400:LEU:HG	1.94	0.50
1:A:259:SER:O	1:A:260:SER:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:PRO:HG3	1:B:450:PHE:CG	2.47	0.49
1:C:324:ILE:HD11	1:C:326:LEU:HD21	1.93	0.49
1:D:258:PRO:C	1:D:260:SER:H	2.15	0.49
1:B:363:ASP:OD1	1:B:366:GLU:HG3	2.13	0.49
1:D:444:ASP:HA	1:D:447:ILE:HD12	1.95	0.49
1:A:436:LEU:HD12	1:A:439:PHE:CD2	2.47	0.49
1:C:255:GLY:HA2	1:C:259:SER:CB	2.43	0.49
1:C:259:SER:O	1:C:261:PRO:N	2.46	0.48
1:A:383:LEU:HD12	1:A:383:LEU:O	2.13	0.48
1:D:326:LEU:HB2	1:D:331:HIS:CD2	2.49	0.48
1:A:280:VAL:HG11	1:C:454:MET:CB	2.44	0.48
1:C:332:VAL:CG2	1:C:337:ALA:HB2	2.43	0.48
1:A:302:ARG:HH12	1:C:448:ASP:CG	2.16	0.48
1:A:449:THR:CG2	1:A:450:PHE:H	2.24	0.48
1:B:268:ILE:HD13	1:B:268:ILE:C	2.34	0.48
1:D:292:LEU:HD12	1:D:388:GLU:OE2	2.12	0.48
1:B:242:VAL:O	1:B:243:GLU:CB	2.62	0.48
1:C:236:LEU:HD13	1:C:236:LEU:O	2.14	0.48
1:A:234:ARG:HG3	2:A:515:HOH:O	2.13	0.48
1:A:304:GLY:O	1:A:308:LEU:HD22	2.14	0.48
1:D:327:ALA:C	1:D:331:HIS:CE1	2.87	0.48
1:A:234:ARG:HA	1:A:237:GLU:HB3	1.96	0.48
1:A:394:GLU:HA	1:A:397:TYR:CE2	2.48	0.48
1:A:452:MET:O	1:A:456:GLU:HB3	2.14	0.48
1:C:338:HIS:O	1:C:340:ALA:N	2.47	0.47
1:B:394:GLU:HA	1:B:397:TYR:CE2	2.48	0.47
1:B:233:GLU:CD	1:B:233:GLU:H	2.18	0.47
1:C:243:GLU:C	1:C:245:LYS:N	2.68	0.47
1:C:411:GLN:HB3	1:C:414:ARG:HB2	1.96	0.47
1:D:287:PRO:O	1:D:288:HIS:HB2	2.14	0.47
1:A:454:MET:HE1	1:C:277:PHE:HB2	1.97	0.47
1:B:236:LEU:O	1:B:236:LEU:HD22	2.15	0.47
1:D:236:LEU:C	1:D:236:LEU:HD13	2.35	0.47
1:B:232:VAL:HG13	1:B:365:THR:CG2	2.45	0.47
1:C:410:GLU:O	1:C:412:PRO:HD3	2.15	0.47
1:C:333:HIS:O	1:C:337:ALA:HB2	2.14	0.47
1:B:264:PRO:O	1:B:268:ILE:HG22	2.15	0.46
1:A:260:SER:C	1:A:262:ASN:H	2.18	0.46
1:A:380:SER:HB2	1:A:383:LEU:HD23	1.96	0.46
1:C:255:GLY:C	1:C:257:ASN:N	2.68	0.46
1:D:439:PHE:CE1	1:D:447:ILE:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ASP:HA	1:B:264:PRO:HD3	1.74	0.46
1:B:322:ASP:OD2	1:B:333:HIS:HD2	1.99	0.46
1:B:422:LEU:HD23	1:B:422:LEU:HA	1.74	0.46
1:C:236:LEU:HD23	1:C:365:THR:HA	1.98	0.46
1:D:325:LEU:HD12	1:D:331:HIS:CE1	2.51	0.46
1:A:260:SER:O	1:A:262:ASN:N	2.42	0.46
1:B:254:MET:O	1:B:255:GLY:C	2.54	0.46
1:D:317:SER:OG	1:D:324:ILE:HA	2.16	0.46
1:A:232:VAL:C	1:A:234:ARG:H	2.20	0.45
1:A:436:LEU:HD12	1:A:439:PHE:HD2	1.81	0.45
1:B:421:ARG:HA	1:B:421:ARG:NE	2.31	0.45
1:A:422:LEU:HD12	1:A:422:LEU:HA	1.78	0.45
1:D:263:ASP:N	1:D:264:PRO:CD	2.80	0.45
1:D:394:GLU:HA	1:D:397:TYR:CE2	2.52	0.45
1:B:248:THR:C	1:B:250:VAL:N	2.69	0.45
1:A:232:VAL:HG11	1:A:365:THR:HG23	1.99	0.45
1:A:299:ILE:HD11	1:A:380:SER:CB	2.41	0.45
1:A:345:ILE:HD11	1:A:428:ILE:HG23	1.99	0.45
1:D:240:LEU:CD2	1:D:364:LYS:HD2	2.47	0.45
1:D:408:TYR:HA	1:D:410:GLU:OE2	2.17	0.45
1:B:265:VAL:HG21	1:D:272:ALA:HB1	1.99	0.45
1:C:447:ILE:O	1:C:451:LEU:HG	2.16	0.45
1:B:288:HIS:HD2	1:B:291:GLU:OE1	2.00	0.45
1:B:353:LEU:O	1:B:357:MET:HG3	2.17	0.45
1:B:415:PHE:CZ	1:B:419:LEU:HD11	2.52	0.45
1:C:317:SER:O	1:C:320:VAL:HG22	2.17	0.44
1:C:348:ARG:HD3	1:D:381:LYS:NZ	2.32	0.44
1:C:421:ARG:NE	1:C:421:ARG:HA	2.32	0.44
1:A:276:LEU:HG	1:C:450:PHE:HE2	1.82	0.44
1:B:330:LEU:HD13	1:B:330:LEU:C	2.38	0.44
1:B:394:GLU:HA	1:B:397:TYR:CD2	2.53	0.44
1:D:325:LEU:HD12	1:D:331:HIS:ND1	2.32	0.44
1:A:421:ARG:HA	1:A:421:ARG:NE	2.32	0.44
1:D:236:LEU:HG	1:D:365:THR:OG1	2.18	0.44
1:C:346:PHE:O	1:C:350:LEU:CD2	2.66	0.43
1:C:403:TYR:OH	1:C:407:LYS:HD3	2.18	0.43
1:B:307:GLU:HG2	1:B:425:LEU:HG	2.00	0.43
1:C:408:TYR:N	1:C:409:PRO:HD3	2.33	0.43
1:C:411:GLN:NE2	1:C:414:ARG:HH11	2.15	0.43
1:A:235:ILE:HD11	1:A:287:PRO:CD	2.41	0.43
1:B:435:HIS:O	1:B:440:LYS:HE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:LEU:O	1:D:280:VAL:HG23	2.18	0.43
1:A:258:PRO:C	1:A:260:SER:H	2.22	0.43
1:D:331:HIS:ND1	1:D:331:HIS:N	2.66	0.43
1:D:434:GLU:HG2	1:D:435:HIS:CD2	2.54	0.43
1:B:323:GLY:HA3	1:B:332:VAL:O	2.18	0.43
1:C:242:VAL:HG21	1:C:278:THR:O	2.19	0.43
1:C:257:ASN:O	1:C:258:PRO:C	2.57	0.43
1:C:337:ALA:O	1:C:338:HIS:C	2.57	0.43
1:A:296:ASP:O	1:A:299:ILE:HG23	2.19	0.42
1:A:274:LYS:NZ	1:A:275:GLN:HE22	2.18	0.42
1:B:310:ILE:HG23	1:B:425:LEU:CD1	2.48	0.42
1:B:318:ILE:HD13	1:B:319:ALA:N	2.35	0.42
1:A:232:VAL:CG1	1:A:365:THR:HG23	2.49	0.42
1:A:452:MET:O	1:A:456:GLU:CB	2.67	0.42
1:B:318:ILE:HD13	1:B:319:ALA:H	1.84	0.42
1:B:451:LEU:O	1:B:455:LEU:HG	2.19	0.42
1:C:360:MET:CE	1:C:418:LEU:HD12	2.48	0.42
1:D:421:ARG:HD2	2:D:524:HOH:O	2.18	0.42
1:C:390:GLU:O	1:C:394:GLU:HG3	2.18	0.42
1:D:439:PHE:HE1	1:D:447:ILE:HD11	1.83	0.42
1:D:457:ALA:HB1	1:D:458:PRO:HD2	2.02	0.42
1:C:452:MET:O	1:C:456:GLU:HA	2.18	0.42
1:A:252:ALA:C	1:A:254:MET:H	2.22	0.42
1:C:236:LEU:O	1:C:240:LEU:HG	2.19	0.42
1:C:295:ASP:O	1:C:299:ILE:HG13	2.19	0.42
1:A:259:SER:O	1:A:260:SER:C	2.58	0.42
1:B:243:GLU:O	1:B:244:PRO:CB	2.68	0.42
1:C:315:HIS:CG	1:C:367:LEU:HD22	2.55	0.42
1:D:417:LYS:NZ	2:D:484:HOH:O	2.52	0.42
1:A:360:MET:HE1	1:A:418:LEU:HD13	2.01	0.42
1:C:236:LEU:HD13	1:C:236:LEU:C	2.40	0.42
1:D:407:LYS:HB3	1:D:408:TYR:CD1	2.54	0.42
1:B:294:LEU:HD23	1:D:452:MET:SD	2.60	0.42
1:B:252:ALA:O	1:B:254:MET:N	2.53	0.41
1:C:279:LEU:HD11	1:C:308:LEU:HB3	2.02	0.41
1:C:348:ARG:O	1:C:352:GLU:HB2	2.20	0.41
1:A:407:LYS:HG2	1:A:408:TYR:CE1	2.54	0.41
1:B:306:ASN:O	1:B:310:ILE:HG22	2.20	0.41
1:A:232:VAL:HA	1:A:235:ILE:HB	2.02	0.41
1:B:252:ALA:C	1:B:254:MET:N	2.73	0.41
1:B:330:LEU:HD22	2:B:480:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:HIS:O	1:C:341:GLY:N	2.44	0.41
1:C:420:LEU:HD13	1:D:393:ARG:HD3	2.02	0.41
1:D:236:LEU:O	1:D:236:LEU:HD22	2.20	0.41
1:D:289:PHE:O	1:D:292:LEU:HB2	2.19	0.41
1:D:334:ARG:HG2	1:D:334:ARG:NH1	2.33	0.41
1:D:324:ILE:O	1:D:331:HIS:HB2	2.20	0.41
1:B:236:LEU:C	1:B:236:LEU:HD13	2.41	0.41
1:C:232:VAL:O	1:C:232:VAL:HG22	2.20	0.41
1:C:255:GLY:O	1:C:257:ASN:N	2.54	0.41
1:C:333:HIS:O	1:C:337:ALA:CB	2.68	0.41
1:C:411:GLN:HE22	1:C:414:ARG:NH1	2.18	0.41
1:D:313:PHE:CE2	1:D:438:PHE:HZ	2.39	0.41
1:B:264:PRO:HB2	1:D:273:ASP:OD1	2.21	0.41
1:B:313:PHE:CD1	1:B:313:PHE:C	2.94	0.41
1:A:315:HIS:CG	1:A:367:LEU:HD22	2.55	0.41
1:A:450:PHE:HA	1:A:453:GLU:CB	2.51	0.41
1:B:301:LEU:HD23	1:B:301:LEU:HA	1.90	0.41
1:C:242:VAL:O	1:C:243:GLU:C	2.59	0.41
1:A:299:ILE:HD12	1:A:383:LEU:HB3	2.04	0.40
1:A:383:LEU:CD1	1:A:386:PRO:HG3	2.50	0.40
1:B:245:LYS:C	1:B:247:GLU:H	2.24	0.40
1:B:310:ILE:HD11	1:B:428:ILE:HG21	2.02	0.40
1:C:453:GLU:O	1:C:456:GLU:HB3	2.21	0.40
1:D:378:PRO:HG3	1:D:390:GLU:OE1	2.22	0.40
1:A:236:LEU:O	1:A:236:LEU:HD13	2.22	0.40
1:A:258:PRO:O	1:A:260:SER:N	2.54	0.40
1:B:435:HIS:O	1:B:436:LEU:HB2	2.21	0.40
1:C:340:ALA:HB1	2:C:496:HOH:O	2.22	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	226/238 (95%)	202 (89%)	14 (6%)	10 (4%)	2 3
1	B	227/238 (95%)	200 (88%)	16 (7%)	11 (5%)	2 2
1	C	224/238 (94%)	193 (86%)	20 (9%)	11 (5%)	2 2
1	D	227/238 (95%)	207 (91%)	13 (6%)	7 (3%)	4 5
All	All	904/952 (95%)	802 (89%)	63 (7%)	39 (4%)	2 3

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	245	LYS
1	A	260	SER
1	A	457	ALA
1	B	243	GLU
1	B	244	PRO
1	B	255	GLY
1	B	264	PRO
1	C	258	PRO
1	C	260	SER
1	C	261	PRO
1	A	244	PRO
1	A	258	PRO
1	B	246	THR
1	B	251	GLU
1	C	244	PRO
1	C	245	LYS
1	C	339	SER
1	D	264	PRO
1	D	327	ALA
1	D	329	GLY
1	A	259	SER
1	B	252	ALA
1	B	258	PRO
1	D	245	LYS
1	A	243	GLU
1	A	254	MET
1	A	264	PRO
1	B	253	ASN
1	B	322	ASP
1	C	256	LEU
1	C	341	GLY
1	D	258	PRO
1	B	260	SER

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Mol	Chain	Res	Type
1	C	334	ARG
1	D	260	SER
1	D	261	PRO
1	C	254	MET
1	C	264	PRO
1	A	261	PRO

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	172/205 (84%)	160 (93%)	12 (7%)	15	29
1	B	176/205 (86%)	164 (93%)	12 (7%)	16	30
1	C	172/205 (84%)	165 (96%)	7 (4%)	30	55
1	D	174/205 (85%)	160 (92%)	14 (8%)	12	23
All	All	694/820 (85%)	649 (94%)	45 (6%)	17	33

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	232	VAL
1	A	299	ILE
1	A	308	LEU
1	A	309	LEU
1	A	353	LEU
1	A	393	ARG
1	A	405	LYS
1	A	418	LEU
1	A	419	LEU
1	A	422	LEU
1	A	445	THR
1	A	455	LEU
1	B	236	LEU
1	B	268	ILE
1	B	312	SER

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Mol	Chain	Res	Type
1	B	318	ILE
1	B	345	ILE
1	B	350	LEU
1	B	385	ASN
1	B	392	LEU
1	B	400	LEU
1	B	436	LEU
1	B	451	LEU
1	B	453	GLU
1	C	301	LEU
1	C	324	ILE
1	C	350	LEU
1	C	370	LEU
1	C	426	ARG
1	C	436	LEU
1	C	453	GLU
1	D	232	VAL
1	D	236	LEU
1	D	306	ASN
1	D	320	VAL
1	D	321	LYS
1	D	345	ILE
1	D	353	LEU
1	D	366	GLU
1	D	410	GLU
1	D	425	LEU
1	D	433	LEU
1	D	434	GLU
1	D	445	THR
1	D	450	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	A	275	GLN
1	A	335	ASN
1	A	338	HIS
1	A	406	HIS
1	B	270	GLN
1	B	288	HIS
1	B	297	GLN

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Mol	Chain	Res	Type
1	B	331	HIS
1	B	333	HIS
1	B	385	ASN
1	C	267	ASN
1	C	270	GLN
1	C	275	GLN
1	C	288	HIS
1	C	297	GLN
1	C	331	HIS
1	C	411	GLN
1	D	267	ASN
1	D	333	HIS
1	D	435	HIS

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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	228/238 (95%)	2.29	58 (25%)	0	0	14, 32, 140, 141	1 (0%)
1	B	229/238 (96%)	1.41	35 (15%)	2	1	14, 28, 121, 139	1 (0%)
1	C	226/238 (94%)	1.77	53 (23%)	0	0	21, 42, 126, 141	0
1	D	229/238 (96%)	1.82	53 (23%)	0	0	17, 39, 131, 134	1 (0%)
All	All	912/952 (95%)	1.82	199 (21%)	0	0	14, 35, 133, 141	3 (0%)

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	253	ASN	24.1
1	B	260	SER	21.2
1	B	261	PRO	20.7
1	A	238	ALA	20.3
1	A	244	PRO	20.2
1	B	254	MET	19.3
1	D	231	PRO	18.1
1	C	248	THR	17.7
1	C	257	ASN	17.3
1	A	231	PRO	17.2
1	A	249	TYR	16.9
1	D	254	MET	16.8
1	C	256	LEU	16.2
1	A	232	VAL	15.8
1	C	258	PRO	15.5
1	D	240	LEU	15.5
1	A	240	LEU	15.4
1	A	458	PRO	15.3
1	B	259	SER	15.0
1	D	256	LEU	14.7
1	A	262	ASN	14.4

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Mol	Chain	Res	Type	RSRZ
1	A	261	PRO	14.2
1	C	245	LYS	14.1
1	B	252	ALA	13.9
1	D	255	GLY	13.8
1	A	248	THR	13.8
1	A	234	ARG	13.8
1	A	245	LYS	13.5
1	A	254	MET	13.4
1	B	255	GLY	13.2
1	C	249	TYR	13.0
1	A	260	SER	12.9
1	D	329	GLY	12.9
1	A	242	VAL	12.8
1	C	260	SER	12.7
1	C	254	MET	12.7
1	A	241	ALA	12.2
1	A	246	THR	12.0
1	C	255	GLY	11.8
1	A	255	GLY	11.5
1	D	246	THR	11.4
1	B	250	VAL	11.3
1	D	248	THR	11.3
1	C	261	PRO	11.2
1	A	235	ILE	11.1
1	B	249	TYR	11.0
1	A	457	ALA	10.7
1	B	258	PRO	10.5
1	A	250	VAL	10.3
1	B	248	THR	10.2
1	C	244	PRO	10.2
1	A	236	LEU	10.0
1	B	242	VAL	10.0
1	D	232	VAL	10.0
1	C	243	GLU	10.0
1	D	247	GLU	9.9
1	D	244	PRO	9.7
1	A	257	ASN	9.6
1	D	241	ALA	9.6
1	C	251	GLU	9.5
1	A	247	GLU	9.3
1	A	258	PRO	9.1
1	D	249	TYR	9.1

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Mol	Chain	Res	Type	RSRZ
1	B	256	LEU	9.1
1	C	340	ALA	9.1
1	B	262	ASN	9.0
1	A	265	VAL	9.0
1	D	328	THR	8.9
1	C	236	LEU	8.9
1	D	242	VAL	8.6
1	B	251	GLU	8.6
1	C	242	VAL	8.6
1	D	234	ARG	8.4
1	A	253	ASN	8.4
1	D	257	ASN	8.3
1	B	231	PRO	8.2
1	C	250	VAL	7.9
1	A	259	SER	7.8
1	C	259	SER	7.8
1	C	246	THR	7.7
1	D	243	GLU	7.7
1	D	252	ALA	7.6
1	A	266	THR	7.6
1	B	246	THR	7.5
1	D	258	PRO	7.4
1	A	233	GLU	7.4
1	D	245	LYS	7.2
1	C	252	ALA	7.1
1	B	244	PRO	7.1
1	A	252	ALA	7.0
1	C	233	GLU	6.9
1	A	251	GLU	6.9
1	B	233	GLU	6.7
1	B	247	GLU	6.6
1	A	237	GLU	6.6
1	D	251	GLU	6.6
1	A	243	GLU	6.5
1	B	458	PRO	6.3
1	D	263	ASP	6.2
1	C	253	ASN	6.2
1	B	257	ASN	6.1
1	D	262	ASN	6.1
1	C	337	ALA	6.0
1	C	232	VAL	6.0
1	D	259	SER	6.0

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Mol	Chain	Res	Type	RSRZ
1	D	261	PRO	6.0
1	D	238	ALA	5.9
1	D	235	ILE	5.9
1	D	233	GLU	5.9
1	D	260	SER	5.8
1	C	237	GLU	5.7
1	B	263	ASP	5.6
1	D	253	ASN	5.6
1	C	240	LEU	5.6
1	B	241	ALA	5.5
1	C	231	PRO	5.4
1	D	250	VAL	5.4
1	D	327	ALA	5.4
1	A	256	LEU	5.3
1	D	236	LEU	5.3
1	D	237	GLU	5.0
1	B	243	GLU	5.0
1	C	339	SER	5.0
1	C	336	SER	4.9
1	B	240	LEU	4.9
1	C	238	ALA	4.9
1	B	232	VAL	4.9
1	B	245	LYS	4.8
1	A	239	GLU	4.8
1	B	235	ILE	4.6
1	C	235	ILE	4.6
1	A	268	ILE	4.5
1	D	266	THR	4.4
1	D	330	LEU	4.3
1	D	444	ASP	4.2
1	A	328	THR	4.2
1	A	270	GLN	4.1
1	C	234	ARG	3.9
1	A	450	PHE	3.9
1	B	238	ALA	3.8
1	C	335	ASN	3.8
1	D	326	LEU	3.8
1	C	247	GLU	3.6
1	D	439	PHE	3.6
1	C	321	LYS	3.5
1	A	444	ASP	3.5
1	D	445	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	237	GLU	3.4
1	C	456	GLU	3.4
1	D	442	ILE	3.4
1	A	455	LEU	3.4
1	C	453	GLU	3.4
1	D	239	GLU	3.4
1	B	234	ARG	3.4
1	C	322	ASP	3.3
1	C	239	GLU	3.3
1	D	324	ILE	3.2
1	A	456	GLU	3.2
1	C	444	ASP	3.1
1	A	327	ALA	3.1
1	A	445	THR	3.0
1	A	375	LEU	3.0
1	C	320	VAL	2.9
1	D	331	HIS	2.9
1	D	441	LEU	2.9
1	C	333	HIS	2.8
1	D	375	LEU	2.8
1	D	267	ASN	2.8
1	D	320	VAL	2.7
1	A	263	ASP	2.7
1	D	265	VAL	2.6
1	B	236	LEU	2.6
1	A	319	ALA	2.6
1	C	338	HIS	2.6
1	A	452	MET	2.6
1	D	294	LEU	2.5
1	C	241	ALA	2.5
1	D	459	HIS	2.5
1	C	328	THR	2.5
1	B	459	HIS	2.4
1	C	442	ILE	2.4
1	D	270	GLN	2.4
1	C	443	GLY	2.3
1	A	449	THR	2.3
1	A	269	CYS	2.3
1	B	239	GLU	2.3
1	A	383	LEU	2.3
1	C	267	ASN	2.3
1	A	384	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	264	PRO	2.2
1	C	451	LEU	2.2
1	A	453	GLU	2.2
1	A	267	ASN	2.2
1	C	449	THR	2.2
1	C	341	GLY	2.2
1	C	348	ARG	2.2
1	A	301	LEU	2.1
1	C	332	VAL	2.1
1	A	300	LEU	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.