



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:03 AM GMT

PDB ID : 4J5X
Title : Crystal Structure of the SR12813-bound PXR/RXRalpha LBD Heterotrimeric Complex
Authors : Wallace, B.D.; Betts, L.; Redinbo, M.R.
Deposited on : 2013-02-10
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

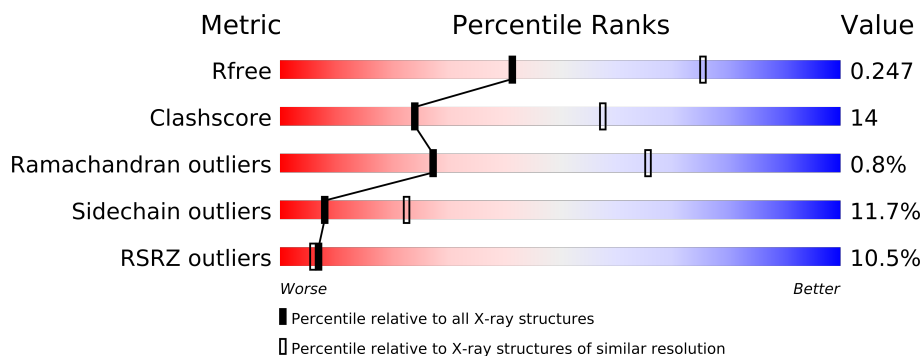
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance





The reported resolution of this entry is 2.80 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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	C	264	
1	D	264	
2	A	336	
2	B	336	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8771 atoms, of which 0 are hydrogen and 0 are deuterium.

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, Nuclear receptor coactivator 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	239	Total	C	N	O	S	0	0	0
			1898	1215	329	343	11			
1	C	238	Total	C	N	O	S	0	0	0
			1887	1210	326	340	11			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	463	GLY	-	LINKER	UNP P19793
D	464	GLY	-	LINKER	UNP P19793
D	465	SER	-	LINKER	UNP P19793
D	466	GLY	-	LINKER	UNP Q15788
D	467	GLY	-	LINKER	UNP Q15788
C	463	GLY	-	LINKER	UNP P19793
C	464	GLY	-	LINKER	UNP P19793
C	465	SER	-	LINKER	UNP P19793
C	466	GLY	-	LINKER	UNP Q15788
C	467	GLY	-	LINKER	UNP Q15788

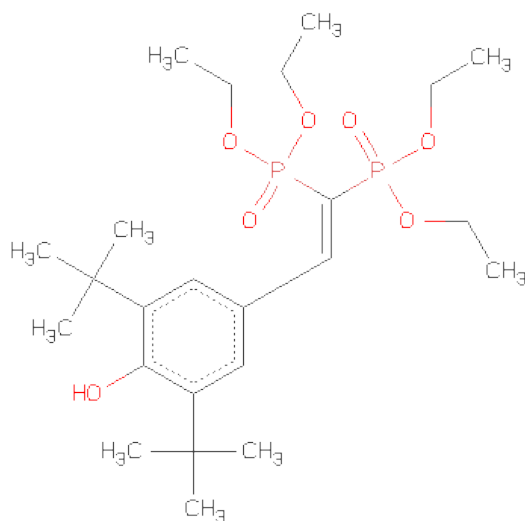
- Molecule 2 is a protein called Nuclear receptor subfamily 1 group I member 2, Nuclear receptor coactivator 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	293	Total	C	N	O	S	0	0	0
			2389	1532	413	426	18			
2	B	293	Total	C	N	O	S	0	0	0
			2371	1519	408	426	18			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	SER	-	EXPRESSION TAG	UNP O75469
A	128	ASN	-	EXPRESSION TAG	UNP O75469
A	129	ALA	-	EXPRESSION TAG	UNP O75469
A	435	GLY	-	LINKER	UNP Q15788
A	436	GLY	-	LINKER	UNP Q15788
A	437	SER	-	LINKER	UNP Q15788
A	438	GLY	-	LINKER	UNP Q15788
A	439	GLY	-	LINKER	UNP Q15788
B	127	SER	-	EXPRESSION TAG	UNP O75469
B	128	ASN	-	EXPRESSION TAG	UNP O75469
B	129	ALA	-	EXPRESSION TAG	UNP O75469
B	435	GLY	-	LINKER	UNP Q15788
B	436	GLY	-	LINKER	UNP Q15788
B	437	SER	-	LINKER	UNP Q15788
B	438	GLY	-	LINKER	UNP Q15788
B	439	GLY	-	LINKER	UNP Q15788

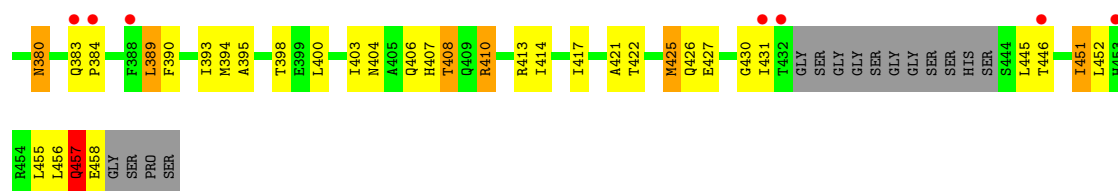
- Molecule 3 is [2-(3,5-DI-TERT-BUTYL-4-HYDROXY-PHENYL)-1-(DIETHOXY-PHOSPHORYL)-VINYL]-PHOSPHONICACID DIETHYL ESTER (three-letter code: SRL) (formula: C₂₄H₄₂O₇P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			33	24	7	2		
3	B	1	Total	C	O	P	0	0
			33	24	7	2		

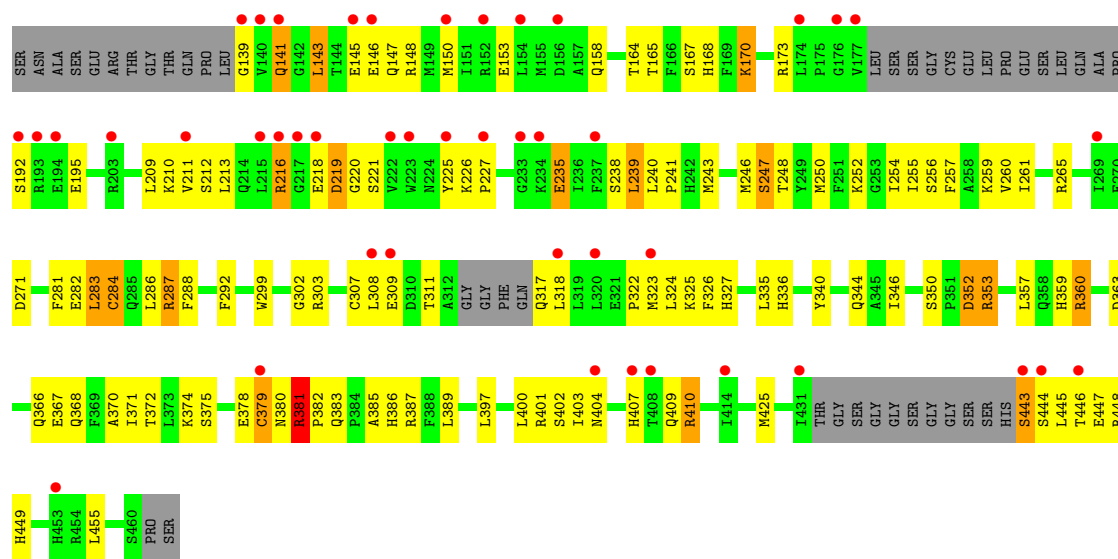
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	44	Total 44	O 44	0	0
4	C	34	Total 34	O 34	0	0
4	A	40	Total 40	O 40	0	0
4	B	42	Total 42	O 42	0	0



- Molecule 2: Nuclear receptor subfamily 1 group I member 2, Nuclear receptor coactivator 1

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.09Å 120.30Å 175.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.65 – 2.80 45.65 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.65-2.80) 99.4 (45.65-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1037)	Depositor
R, R_{free}	0.245 , 0.298 0.249 , 0.247	Depositor DCC
R_{free} test set	1849 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.852	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 26.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 37160 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8771	wwPDB-VP
Average B, all atoms (Å ²)	54.0	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 35.15 % 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 6.1035e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SRL

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	C	0.23	0/1924	0.42	0/2599
1	D	0.25	0/1935	0.44	0/2614
2	A	0.27	0/2440	0.52	0/3283
2	B	0.28	0/2420	0.50	0/3257
All	All	0.26	0/8719	0.48	0/11753

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1887	0	1926	34	1
1	D	1898	0	1936	38	1
2	A	2389	0	2402	82	0
2	B	2371	0	2374	98	0
3	A	33	0	42	3	0
3	B	33	0	42	18	0
4	A	40	0	0	14	0
4	B	42	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	34	0	0	1	0
4	D	44	0	0	9	0
All	All	8771	0	8722	246	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (246) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:209:LEU:HB3	3:B:501:SRL:H301	1.52	0.89
3:A:501:SRL:H233	3:A:501:SRL:H173	1.55	0.87
2:B:282:GLU:HG3	2:B:404:ASN:HD22	1.44	0.83
1:D:352:GLU:HG2	2:A:352:ASP:HB3	1.64	0.79
2:A:237:PHE:O	2:A:241:PRO:HD3	1.84	0.78
2:A:216:ARG:NH2	2:A:305:SER:OG	2.21	0.74
1:C:420:LEU:HD11	2:B:366:GLN:HG2	1.69	0.74
2:B:344:GLN:HG2	4:B:641:HOH:O	1.88	0.72
1:D:237:GLU:OE2	4:D:533:HOH:O	2.07	0.71
1:D:352:GLU:OE2	2:A:359:HIS:NE2	2.21	0.70
2:B:212:SER:HB2	2:B:307:CYS:HB3	1.73	0.70
2:B:254:ILE:HD12	2:B:283:LEU:HB3	1.77	0.67
1:C:352:GLU:HG2	2:B:352:ASP:HB3	1.74	0.67
2:B:216:ARG:NH1	2:B:303:ARG:O	2.28	0.67
2:B:283:LEU:HA	4:B:641:HOH:O	1.94	0.67
2:B:209:LEU:HB3	3:B:501:SRL:C30	2.25	0.67
2:A:264:PHE:O	2:A:272:GLN:NE2	2.28	0.66
2:B:173:ARG:HE	2:B:241:PRO:HB2	1.59	0.66
3:B:501:SRL:HC6	3:B:501:SRL:O28	1.96	0.66
2:A:390:PHE:H	2:A:393:ILE:HD12	1.61	0.65
2:A:425:MET:HE2	4:A:639:HOH:O	1.96	0.65
1:C:476:ARG:NH1	1:C:477:HIS:O	2.29	0.65
2:A:281:PHE:HE2	2:A:403:ILE:HG22	1.61	0.65
2:B:374:LYS:NZ	4:B:618:HOH:O	2.29	0.65
2:A:383:GLN:HB2	2:A:384:PRO:HD3	1.77	0.65
1:D:348:ARG:NH1	2:A:352:ASP:O	2.30	0.65
1:C:448:ASP:OD1	1:C:448:ASP:N	2.29	0.65
1:C:263:ASP:OD2	1:C:266:THR:OG1	2.16	0.64
1:C:302:ARG:HD2	1:C:477:HIS:CD2	2.33	0.64
1:D:393:ARG:NH2	4:D:515:HOH:O	2.30	0.63
1:D:482:ARG:NH1	4:D:526:HOH:O	2.31	0.62
2:A:353:ARG:NH1	4:A:604:HOH:O	2.31	0.62
2:A:318:LEU:HB3	2:A:324:LEU:HD22	1.82	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:342:LEU:HD23	4:A:634:HOH:O	2.00	0.62
1:C:239:GLU:OE1	1:C:371:ARG:NH1	2.33	0.62
2:B:383:GLN:O	2:B:385:ALA:N	2.31	0.61
2:B:139:GLY:HA2	2:B:382:PRO:HD2	1.82	0.60
2:B:219:ASP:OD1	2:B:220:GLY:N	2.35	0.60
2:B:243:MET:O	2:B:247:SER:OG	2.20	0.60
2:B:281:PHE:HE2	2:B:403:ILE:HG22	1.66	0.60
2:B:210:LYS:HE2	2:B:227:PRO:HB2	1.84	0.60
2:B:326:PHE:HB2	2:B:403:ILE:HD11	1.84	0.59
3:B:501:SRL:H291	3:B:501:SRL:H153	1.83	0.59
2:B:282:GLU:HG2	2:B:400:LEU:HG	1.85	0.59
2:A:236:ILE:HD12	2:A:236:ILE:H	1.67	0.59
2:B:260:VAL:O	4:B:628:HOH:O	2.16	0.59
1:D:371:ARG:HD2	4:D:538:HOH:O	2.02	0.58
2:A:345:ALA:HB3	4:A:634:HOH:O	2.04	0.58
1:D:411:GLN:NE2	4:D:536:HOH:O	2.36	0.58
2:A:143:LEU:HB2	2:A:148:ARG:HG3	1.85	0.57
2:B:307:CYS:SG	2:B:308:LEU:N	2.77	0.57
1:C:243:GLU:OE2	1:C:316:ARG:NH1	2.33	0.57
2:B:283:LEU:HD12	4:B:641:HOH:O	2.03	0.57
2:B:381:ARG:O	2:B:383:GLN:N	2.35	0.57
1:D:345:ILE:HD13	1:D:431:LYS:HB3	1.84	0.57
2:A:209:LEU:HD13	3:A:501:SRL:H301	1.86	0.57
2:A:342:LEU:HA	4:A:634:HOH:O	2.03	0.57
1:D:323:GLY:O	4:D:505:HOH:O	2.18	0.56
2:B:284:CYS:HG	2:B:288:PHE:HE2	1.54	0.56
2:A:311:THR:OG1	2:A:312:ALA:N	2.37	0.56
2:B:425:MET:CE	3:B:501:SRL:H191	2.36	0.55
2:A:278:GLY:HA3	2:A:353:ARG:HD2	1.89	0.55
1:D:334:ARG:HB3	1:D:346:PHE:CE2	2.41	0.55
1:D:294:LEU:HD21	1:D:485:GLN:HG2	1.87	0.55
1:C:302:ARG:HH11	1:C:477:HIS:CD2	2.24	0.55
2:B:407:HIS:CE1	2:B:410:ARG:HH11	2.25	0.55
2:A:316:GLN:OE1	2:A:317:GLN:N	2.39	0.55
2:B:380:ASN:OD1	2:B:381:ARG:N	2.40	0.54
2:B:235:GLU:O	2:B:238:SER:OG	2.26	0.54
2:B:141:GLN:HE22	2:B:380:ASN:HD22	1.54	0.54
2:B:256:SER:HA	2:B:259:LYS:HB2	1.89	0.54
2:B:360:ARG:NH1	2:B:363:ASP:OD2	2.41	0.54
2:B:286:LEU:HB2	4:B:641:HOH:O	2.07	0.54
2:A:353:ARG:O	2:A:356:VAL:HG12	2.08	0.53
2:A:270:GLU:HG2	2:A:445:LEU:HD13	1.89	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:323:MET:HB2	2:B:407:HIS:HE2	1.74	0.53
1:D:294:LEU:HG	4:D:542:HOH:O	2.08	0.52
2:B:211:VAL:HG12	2:B:307:CYS:O	2.10	0.52
2:B:158:GLN:OE1	2:B:287:ARG:NH1	2.42	0.52
2:A:351:PRO:HG3	2:A:363:ASP:HA	1.92	0.52
1:D:310:ILE:HA	1:D:313:PHE:CD2	2.44	0.52
2:B:445:LEU:O	2:B:449:HIS:N	2.36	0.52
2:B:170:LYS:NZ	4:B:620:HOH:O	2.35	0.52
2:A:352:ASP:OD1	2:A:352:ASP:N	2.41	0.52
2:A:239:LEU:O	2:A:243:MET:HG2	2.10	0.52
2:B:340:TYR:O	2:B:344:GLN:HG3	2.09	0.52
2:A:238:SER:O	2:A:241:PRO:HD2	2.10	0.52
1:C:323:GLY:HA2	1:C:346:PHE:HZ	1.75	0.52
2:A:267:LEU:HB3	4:A:632:HOH:O	2.10	0.52
2:B:146:GLU:OE2	4:B:633:HOH:O	2.19	0.51
2:A:206:LEU:HB3	2:A:236:ILE:HG21	1.91	0.51
2:B:265:ARG:NH2	4:B:628:HOH:O	2.25	0.51
1:C:421:ARG:NH1	4:C:516:HOH:O	2.43	0.51
2:B:139:GLY:HA2	2:B:382:PRO:CD	2.40	0.51
2:B:213:LEU:HB3	2:B:225:TYR:HB3	1.93	0.51
1:D:434:GLU:OE2	4:D:518:HOH:O	2.19	0.50
2:A:244:ALA:O	2:A:247:SER:OG	2.20	0.50
2:B:165:THR:HG1	2:B:167:SER:HG	1.54	0.50
1:C:417:LYS:HE2	2:B:367:GLU:HB3	1.92	0.50
1:C:345:ILE:HD13	1:C:431:LYS:HB3	1.92	0.50
2:A:270:GLU:HG2	2:A:445:LEU:HB3	1.94	0.49
2:B:147:GLN:HB3	2:B:372:THR:HG23	1.94	0.49
2:A:270:GLU:CG	2:A:445:LEU:HB3	2.43	0.49
1:D:310:ILE:HA	1:D:313:PHE:CE2	2.47	0.49
1:C:310:ILE:HA	1:C:313:PHE:CE2	2.47	0.49
2:B:363:ASP:O	2:B:367:GLU:HG3	2.12	0.49
1:C:423:PRO:HB2	2:B:401:ARG:HD2	1.94	0.49
2:B:327:HIS:CD2	3:B:501:SRL:H263	2.47	0.49
2:A:173:ARG:HE	2:A:241:PRO:HB3	1.78	0.49
1:C:453:GLU:CD	1:C:477:HIS:HA	2.33	0.49
2:B:346:ILE:HG21	2:B:397:LEU:HD13	1.93	0.49
2:B:247:SER:OG	3:B:501:SRL:H171	2.13	0.49
2:A:456:LEU:O	2:A:457:GLN:HB3	2.12	0.49
2:A:234:LYS:HA	2:A:237:PHE:CD2	2.48	0.48
2:B:425:MET:HE1	3:B:501:SRL:H191	1.94	0.48
1:D:264:PRO:O	1:D:268:ILE:HG13	2.13	0.48
2:B:407:HIS:HA	2:B:410:ARG:HB2	1.94	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:143:LEU:HD23	2:B:379:CYS:SG	2.53	0.48
2:B:447:GLU:HG2	2:B:448:ARG:N	2.29	0.48
2:B:443:SER:HB2	2:B:448:ARG:HE	1.79	0.47
1:D:401:GLU:HG2	1:D:405:LYS:HE2	1.96	0.47
2:B:381:ARG:N	2:B:382:PRO:HD3	2.29	0.47
1:D:447:ILE:HG23	1:D:451:LEU:HD23	1.97	0.47
2:B:299:TRP:CD2	3:B:501:SRL:H222	2.49	0.47
2:B:352:ASP:OD1	2:B:352:ASP:N	2.25	0.47
1:C:266:THR:HG23	1:C:446:PRO:HD2	1.97	0.47
2:B:281:PHE:CE2	2:B:403:ILE:HG22	2.48	0.47
2:A:207:CYS:SG	2:A:208:SER:N	2.88	0.47
2:A:158:GLN:O	2:A:162:PHE:N	2.48	0.47
2:A:426:GLN:O	2:A:430:GLY:N	2.48	0.47
1:D:345:ILE:O	1:D:349:VAL:HG23	2.15	0.46
2:A:426:GLN:HG2	2:A:431:ILE:HB	1.96	0.46
2:A:164:THR:HG23	4:A:640:HOH:O	2.14	0.46
1:C:323:GLY:HA2	1:C:346:PHE:CZ	2.50	0.46
2:A:406:GLN:O	2:A:410:ARG:HB2	2.14	0.46
2:A:202:VAL:HG13	2:A:414:ILE:HG12	1.96	0.46
2:B:282:GLU:HG3	2:B:404:ASN:ND2	2.23	0.46
1:C:426:ARG:HH11	2:B:402:SER:HG	1.64	0.46
2:A:395:ALA:O	2:A:398:THR:OG1	2.30	0.46
2:A:223:TRP:CZ3	2:B:225:TYR:HB2	2.51	0.46
2:A:377:ILE:HG21	2:A:389:LEU:HB3	1.97	0.46
2:B:367:GLU:O	2:B:371:ILE:HG13	2.16	0.46
1:D:298:VAL:HG13	1:D:480:LEU:HD13	1.98	0.46
2:A:255:ILE:HG22	2:A:456:LEU:HD21	1.97	0.45
2:B:368:GLN:O	2:B:372:THR:OG1	2.26	0.45
1:C:476:ARG:HB2	1:C:477:HIS:H	1.41	0.45
2:A:271:ASP:HB2	4:A:632:HOH:O	2.15	0.45
2:B:443:SER:O	2:B:448:ARG:NH1	2.49	0.45
2:B:322:PRO:HA	2:B:325:LYS:HB3	1.99	0.45
2:A:451:ILE:O	2:A:455:LEU:HG	2.17	0.45
2:B:407:HIS:CE1	3:B:501:SRL:H141	2.52	0.45
2:B:141:GLN:NE2	2:B:380:ASN:HD22	2.13	0.45
2:A:156:ASP:O	2:A:160:LYS:HB2	2.17	0.45
2:A:421:ALA:HA	4:A:639:HOH:O	2.15	0.45
1:D:367:LEU:HD11	4:D:538:HOH:O	2.17	0.45
2:A:141:GLN:HG2	2:A:142:GLY:N	2.31	0.45
1:D:356:LYS:HD3	1:D:356:LYS:HA	1.68	0.45
1:D:277:PHE:O	1:D:281:GLU:HG2	2.17	0.45
2:A:349:PHE:O	2:A:366:GLN:HB2	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:302:ARG:HD2	1:C:477:HIS:NE2	2.31	0.45
2:B:346:ILE:HD11	2:B:370:ALA:HA	1.98	0.45
1:D:245:LYS:O	1:D:245:LYS:NZ	2.40	0.45
2:B:299:TRP:CG	3:B:501:SRL:H222	2.51	0.45
2:A:141:GLN:HG2	2:A:142:GLY:H	1.81	0.44
2:B:250:MET:O	2:B:254:ILE:HG12	2.17	0.44
2:B:254:ILE:HG23	2:B:283:LEU:HD23	2.00	0.44
2:A:269:ILE:HD12	2:A:270:GLU:H	1.82	0.44
3:B:501:SRL:C29	3:B:501:SRL:H142	2.48	0.44
2:B:239:LEU:HD11	4:B:639:HOH:O	2.18	0.44
2:A:260:VAL:O	2:A:265:ARG:NH2	2.50	0.44
2:B:252:LYS:HA	2:B:255:ILE:HD12	1.99	0.44
2:B:212:SER:OG	2:B:309:GLU:OE1	2.23	0.44
2:B:326:PHE:HB2	2:B:403:ILE:CD1	2.47	0.44
2:A:422:THR:OG1	2:A:425:MET:HB2	2.18	0.44
2:B:299:TRP:CZ2	3:B:501:SRL:H262	2.53	0.44
2:A:216:ARG:HG2	2:A:222:VAL:HG22	1.99	0.44
1:D:448:ASP:N	1:D:448:ASP:OD1	2.42	0.44
2:B:219:ASP:OD1	2:B:221:SER:OG	2.31	0.44
1:C:414:ARG:O	1:C:418:LEU:HG	2.18	0.44
1:C:310:ILE:HA	1:C:313:PHE:CD2	2.52	0.43
2:A:218:GLU:HG2	2:A:218:GLU:H	1.66	0.43
2:A:282:GLU:HG3	2:A:400:LEU:HD22	1.99	0.43
1:C:302:ARG:HH11	1:C:477:HIS:HD2	1.64	0.43
2:A:281:PHE:CE2	2:A:403:ILE:HG22	2.46	0.43
1:C:301:LEU:O	1:C:305:TRP:HB3	2.19	0.43
1:C:387:ALA:HA	1:C:390:GLU:HB3	2.00	0.43
2:B:292:PHE:HD1	2:B:299:TRP:CE2	2.37	0.43
2:B:292:PHE:CD1	2:B:299:TRP:CE2	3.07	0.43
1:C:334:ARG:HB3	1:C:346:PHE:CE2	2.54	0.43
1:D:257:ASN:N	1:D:257:ASN:OD1	2.52	0.42
2:A:205:ASP:CG	2:A:413:ARG:HH21	2.22	0.42
2:A:456:LEU:HD22	4:A:638:HOH:O	2.18	0.42
1:D:347:ASP:O	1:D:351:THR:HG23	2.18	0.42
2:B:218:GLU:H	2:B:218:GLU:CD	2.22	0.42
2:A:267:LEU:HD22	4:A:632:HOH:O	2.19	0.42
2:A:212:SER:HB2	4:A:626:HOH:O	2.18	0.42
1:C:298:VAL:HG13	1:C:480:LEU:HD13	2.01	0.42
2:A:335:LEU:HB2	2:A:340:TYR:CE2	2.54	0.42
2:A:213:LEU:HB3	2:A:225:TYR:HB3	2.01	0.42
2:B:145:GLU:HA	2:B:148:ARG:HD3	2.01	0.42
2:A:452:LEU:HA	2:A:452:LEU:HD12	1.86	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:276:LEU:HD21	1:D:305:TRP:CE3	2.54	0.42
2:B:286:LEU:HD12	4:B:641:HOH:O	2.19	0.42
1:C:356:LYS:HA	1:C:356:LYS:HD3	1.79	0.42
2:B:407:HIS:HB3	3:B:501:SRL:H162	2.01	0.42
2:B:407:HIS:ND1	3:B:501:SRL:H141	2.35	0.42
1:D:310:ILE:HD12	1:D:429:GLY:HA2	2.00	0.42
2:B:336:HIS:CE1	2:B:381:ARG:HH11	2.38	0.42
2:A:291:VAL:HG13	4:A:640:HOH:O	2.20	0.42
2:A:248:THR:O	2:A:252:LYS:HB2	2.19	0.42
2:A:269:ILE:HG13	2:A:269:ILE:H	1.53	0.41
2:B:375:SER:HA	2:B:378:GLU:HB3	2.01	0.41
1:C:370:LEU:HD23	1:C:370:LEU:HA	1.86	0.41
2:A:298:THR:HB	2:A:307:CYS:HA	2.02	0.41
2:A:367:GLU:O	2:A:371:ILE:HG12	2.19	0.41
2:A:380:ASN:OD1	2:A:380:ASN:N	2.53	0.41
1:C:297:GLN:HB2	1:C:484:LEU:HD13	2.03	0.41
2:B:383:GLN:O	2:B:386:HIS:N	2.53	0.41
1:D:323:GLY:HA3	1:D:332:VAL:O	2.20	0.41
1:D:297:GLN:HB2	1:D:484:LEU:HD13	2.01	0.41
2:A:251:PHE:O	2:A:255:ILE:HG13	2.21	0.41
2:A:394:MET:O	2:A:398:THR:HG23	2.20	0.41
2:B:248:THR:O	2:B:252:LYS:HG2	2.20	0.41
2:B:350:SER:O	2:B:353:ARG:HG3	2.20	0.41
2:B:288:PHE:CD1	3:B:501:SRL:H221	2.56	0.41
1:D:301:LEU:O	1:D:305:TRP:HB3	2.20	0.41
1:D:234:ARG:HB3	1:D:234:ARG:HE	1.54	0.41
2:B:335:LEU:HB2	2:B:340:TYR:CE2	2.56	0.41
1:C:348:ARG:O	1:C:352:GLU:HB2	2.20	0.41
2:A:407:HIS:CE1	3:A:501:SRL:H183	2.55	0.41
1:C:352:GLU:CD	2:B:359:HIS:HE2	2.23	0.41
1:D:423:PRO:N	2:A:398:THR:HG22	2.36	0.41
1:C:445:THR:O	1:C:447:ILE:HG13	2.20	0.41
2:A:404:ASN:O	2:A:408:THR:OG1	2.38	0.41
1:D:289:PHE:CD1	1:D:375:LEU:HD21	2.55	0.41
1:D:366:GLU:OE2	1:D:414:ARG:NH2	2.49	0.41
2:A:264:PHE:HE1	4:A:638:HOH:O	2.03	0.41
2:B:425:MET:HE2	3:B:501:SRL:H191	2.03	0.40
2:B:283:LEU:HD12	2:B:283:LEU:HA	1.93	0.40
2:B:165:THR:O	2:B:302:GLY:HA3	2.21	0.40
2:A:202:VAL:HG11	2:A:417:ILE:HD11	2.03	0.40
1:D:306:ASN:O	1:D:310:ILE:HG13	2.21	0.40
2:B:257:PHE:O	2:B:261:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:501:SRL:H291	3:B:501:SRL:H142	2.03	0.40
2:A:315:PHE:HD1	2:A:315:PHE:HA	1.73	0.40
2:A:261:ILE:O	2:A:265:ARG:HG3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:247:GLU:OE2	1:C:248:THR:OG1[1.665]	2.13	0.07

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	C	232/264 (88%)	220 (95%)	10 (4%)	2 (1%)	25	63
1	D	233/264 (88%)	222 (95%)	10 (4%)	1 (0%)	43	80
2	A	287/336 (85%)	263 (92%)	22 (8%)	2 (1%)	30	69
2	B	285/336 (85%)	253 (89%)	29 (10%)	3 (1%)	21	57
All	All	1037/1200 (86%)	958 (92%)	71 (7%)	8 (1%)	27	65

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	457	GLN
2	B	219	ASP
2	B	381	ARG
1	C	263	ASP
2	A	311	THR
2	B	141	GLN
1	D	263	ASP
1	C	342	VAL

5.3.2 Protein sidechains ⓘ

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	C	205/227 (90%)	184 (90%)	21 (10%)	11	29
1	D	207/227 (91%)	184 (89%)	23 (11%)	9	25
2	A	262/295 (89%)	234 (89%)	28 (11%)	10	26
2	B	260/295 (88%)	223 (86%)	37 (14%)	5	14
All	All	934/1044 (90%)	825 (88%)	109 (12%)	8	22

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	229	ASP
1	D	230	MET
1	D	232	VAL
1	D	234	ARG
1	D	245	LYS
1	D	256	LEU
1	D	257	ASN
1	D	313	PHE
1	D	320	VAL
1	D	338	HIS
1	D	348	ARG
1	D	352	GLU
1	D	362	MET
1	D	363	ASP
1	D	381	LYS
1	D	384	SER
1	D	404	CYS
1	D	407	LYS
1	D	420	LEU
1	D	448	ASP
1	D	450	PHE
1	D	476	ARG
1	D	480	LEU
1	C	228	GLU
1	C	229	ASP
1	C	230	MET

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Mol	Chain	Res	Type
1	C	232	VAL
1	C	240	LEU
1	C	245	LYS
1	C	256	LEU
1	C	266	THR
1	C	313	PHE
1	C	324	ILE
1	C	348	ARG
1	C	352	GLU
1	C	362	MET
1	C	363	ASP
1	C	420	LEU
1	C	448	ASP
1	C	450	PHE
1	C	476	ARG
1	C	477	HIS
1	C	478	LYS
1	C	480	LEU
2	A	143	LEU
2	A	153	GLU
2	A	156	ASP
2	A	159	MET
2	A	160	LYS
2	A	168	HIS
2	A	213	LEU
2	A	269	ILE
2	A	298	THR
2	A	303	ARG
2	A	308	LEU
2	A	311	THR
2	A	315	PHE
2	A	316	GLN
2	A	323	MET
2	A	329	MET
2	A	358	GLN
2	A	371	ILE
2	A	380	ASN
2	A	389	LEU
2	A	408	THR
2	A	410	ARG
2	A	425	MET
2	A	427	GLU

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Mol	Chain	Res	Type
2	A	446	THR
2	A	451	ILE
2	A	457	GLN
2	A	458	GLU
2	B	143	LEU
2	B	150	MET
2	B	153	GLU
2	B	164	THR
2	B	168	HIS
2	B	170	LYS
2	B	192	SER
2	B	195	GLU
2	B	216	ARG
2	B	226	LYS
2	B	235	GLU
2	B	239	LEU
2	B	240	LEU
2	B	246	MET
2	B	247	SER
2	B	271	ASP
2	B	283	LEU
2	B	284	CYS
2	B	287	ARG
2	B	311	THR
2	B	317	GLN
2	B	318	LEU
2	B	324	LEU
2	B	352	ASP
2	B	353	ARG
2	B	357	LEU
2	B	360	ARG
2	B	379	CYS
2	B	381	ARG
2	B	387	ARG
2	B	389	LEU
2	B	409	GLN
2	B	410	ARG
2	B	443	SER
2	B	444	SER
2	B	446	THR
2	B	455	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	D	262	ASN
1	C	477	HIS
2	A	141	GLN
2	B	141	GLN
2	B	201	GLN
2	B	404	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SRL	A	501	-	33,33,33	1.27	5 (15%)	49,50,50	1.99	16 (32%)
3	SRL	B	501	-	33,33,33	1.60	6 (18%)	49,50,50	2.03	15 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SRL	A	501	-	-	6/44/44/44	0/1/1/1
3	SRL	B	501	-	-	2/44/44/44	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	SRL	C13-C3	-4.11	1.47	1.54
3	B	501	SRL	P10-O27	4.04	1.51	1.46
3	B	501	SRL	C4-C5	-3.08	1.34	1.39
3	B	501	SRL	P9-O24	2.88	1.64	1.57
3	A	501	SRL	P10-O27	2.81	1.50	1.46
3	A	501	SRL	P9-O20	2.69	1.49	1.46
3	A	501	SRL	P10-C8	2.42	1.83	1.79
3	B	501	SRL	C5-C7	2.38	1.51	1.46
3	B	501	SRL	C12-C1	-2.27	1.50	1.54
3	A	501	SRL	C13-C3	-2.15	1.50	1.54
3	A	501	SRL	C5-C7	2.09	1.51	1.46

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	SRL	C4-C3-C2	6.59	122.91	116.77
3	B	501	SRL	C3-C2-C1	-5.57	116.89	122.66
3	A	501	SRL	C5-C7-C8	-4.89	120.35	131.07
3	A	501	SRL	O31-P10-O27	-4.41	105.37	115.07
3	A	501	SRL	O24-P9-O21	3.65	112.00	101.66
3	A	501	SRL	O20-P9-C8	-3.35	106.19	113.81
3	B	501	SRL	C12-C1-C2	3.35	125.33	121.96
3	B	501	SRL	O24-P9-C8	3.27	115.75	104.97
3	A	501	SRL	C3-C2-C1	-3.23	119.32	122.66
3	A	501	SRL	C12-C1-C2	3.16	125.14	121.96
3	A	501	SRL	C4-C3-C2	3.15	119.70	116.77
3	A	501	SRL	O21-P9-C8	2.94	114.66	104.97
3	A	501	SRL	O28-P10-O27	-2.91	108.68	115.07
3	B	501	SRL	O28-P10-O27	-2.83	108.84	115.07
3	A	501	SRL	C16-C12-C1	2.77	116.33	110.91
3	B	501	SRL	O20-P9-C8	-2.71	107.64	113.81
3	B	501	SRL	C16-C12-C1	2.69	116.17	110.91
3	A	501	SRL	O31-P10-O28	2.63	109.13	101.66
3	B	501	SRL	O31-P10-C8	2.59	113.50	104.97
3	B	501	SRL	C19-C13-C3	-2.47	106.08	110.91
3	A	501	SRL	O21-P9-O20	-2.43	109.71	115.07
3	A	501	SRL	O28-P10-C8	2.41	112.89	104.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	SRL	O28-P10-C8	-2.30	97.38	104.97
3	B	501	SRL	C15-C12-C1	-2.18	106.64	110.91
3	B	501	SRL	O31-P10-O28	2.15	107.77	101.66
3	A	501	SRL	P9-O21-C22	-2.15	116.16	122.04
3	B	501	SRL	O24-P9-O21	2.12	107.68	101.66
3	B	501	SRL	C6-C5-C7	2.09	128.11	120.92
3	B	501	SRL	C4-C3-C13	-2.08	114.47	119.93
3	A	501	SRL	C6-C1-C2	2.07	118.70	116.77
3	A	501	SRL	O27-P10-C8	-2.05	109.14	113.81

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	SRL	O27-P10-C8-C7
3	B	501	SRL	O31-P10-C8-P9
3	A	501	SRL	O24-P9-C8-P10
3	A	501	SRL	O28-P10-C8-C7
3	A	501	SRL	P9-C8-C7-C5
3	B	501	SRL	O21-P9-C8-P10
3	A	501	SRL	O31-P10-C8-P9
3	A	501	SRL	O20-P9-C8-P10

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	C	238/264 (90%)	0.56	17 (7%)	16 14	28, 47, 73, 123	0
1	D	239/264 (90%)	0.44	12 (5%)	28 28	30, 46, 79, 101	0
2	A	293/336 (87%)	0.84	37 (12%)	4 3	28, 54, 90, 128	0
2	B	293/336 (87%)	0.94	44 (15%)	3 2	33, 55, 93, 111	0
All	All	1063/1200 (88%)	0.72	110 (10%)	7 6	28, 51, 87, 128	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	211	VAL	6.5
2	A	177	VAL	5.8
2	B	177	VAL	5.8
2	B	211	VAL	5.5
1	D	477	HIS	5.5
2	B	176	GLY	5.2
2	A	237	PHE	5.0
2	B	141	GLN	4.8
2	B	443	SER	4.8
2	A	230	ASP	4.7
2	B	446	THR	4.3
2	B	192	SER	4.2
2	B	233	GLY	4.2
2	A	209	LEU	4.1
2	B	234	LYS	4.1
2	B	318	LEU	4.1
2	A	384	PRO	4.1
2	A	233	GLY	3.8
2	A	210	LYS	3.7
2	A	235	GLU	3.7
2	B	174	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	269	ILE	3.6
2	A	212	SER	3.6
2	B	227	PRO	3.6
2	B	193	ARG	3.6
2	B	215	LEU	3.5
2	B	237	PHE	3.5
2	B	140	VAL	3.4
1	C	262	ASN	3.4
2	A	207	CYS	3.4
2	A	383	GLN	3.3
2	A	308	LEU	3.3
2	B	154	LEU	3.2
1	D	366	GLU	3.2
1	C	456	GLU	3.2
2	A	199	TRP	3.1
2	B	320	LEU	3.1
1	D	263	ASP	3.1
2	B	156	ASP	3.1
2	A	266	ASP	3.1
2	A	193	ARG	3.0
2	B	309	GLU	3.0
2	A	313	GLY	3.0
2	B	217	GLY	3.0
1	D	476	ARG	2.9
1	C	263	ASP	2.9
2	A	174	LEU	2.9
2	B	146	GLU	2.9
2	A	388	PHE	2.9
2	A	453	HIS	2.9
2	B	444	SER	2.9
2	B	218	GLU	2.8
1	C	413	GLY	2.8
2	A	141	GLN	2.8
1	C	458	PRO	2.7
2	A	231	SER	2.7
2	A	314	GLY	2.7
1	D	373	ILE	2.7
2	A	315	PHE	2.7
1	C	247	GLU	2.7
2	B	150	MET	2.6
1	D	441	LEU	2.6
2	A	240	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	A	145	GLU	2.6
2	B	404	ASN	2.6
1	C	441	LEU	2.5
2	B	453	HIS	2.5
2	B	152	ARG	2.5
2	A	432	THR	2.5
2	B	194	GLU	2.5
1	C	285	ARG	2.5
2	B	203	ARG	2.5
2	B	145	GLU	2.5
2	B	407	HIS	2.5
1	C	236	LEU	2.5
2	A	267	LEU	2.5
1	C	235	ILE	2.4
2	A	431	ILE	2.4
1	C	476	ARG	2.4
1	D	311	ALA	2.4
2	A	446	THR	2.4
1	D	257	ASN	2.4
1	C	232	VAL	2.3
2	B	225	TYR	2.3
1	D	444	ASP	2.3
2	B	431	ILE	2.3
2	A	150	MET	2.3
2	B	222	VAL	2.3
2	B	379	CYS	2.3
2	B	414	ILE	2.3
2	B	216	ARG	2.3
2	B	223	TRP	2.2
2	B	408	THR	2.2
2	A	227	PRO	2.2
1	C	424	ALA	2.2
2	B	323	MET	2.2
2	A	302	GLY	2.2
1	C	427	SER	2.2
1	C	477	HIS	2.1
1	C	290	SER	2.1
2	B	308	LEU	2.1
2	A	260	VAL	2.1
1	D	418	LEU	2.1
2	A	176	GLY	2.1
1	C	248	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	245	LYS	2.0
2	A	232	GLY	2.0
2	B	139	GLY	2.0
1	D	364	LYS	2.0
2	A	225	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SRL	B	501	33/33	0.43	1.71	56,88,109,114	0
3	SRL	A	501	33/33	0.43	1.26	57,80,95,114	0

6.5 Other polymers

There are no such residues in this entry.