Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:36 AM GMT

PDB ID	:	3FAL
Title	:	humanRXR alpha & mouse LXR alpha complexed with Retenoic acid and GSK2186
Authors	:	Chao, E.Y.; Caravella, J.A.; Watson, M.A.; Campobasso, N.; Ghisletti, S.; Billin, A.N.; Galardi, C.; Willson, T.M.; Zuercher, W.J.; Collins, J.L.
Deposited on	:	2008-11-17
Resolution	:	2.36 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

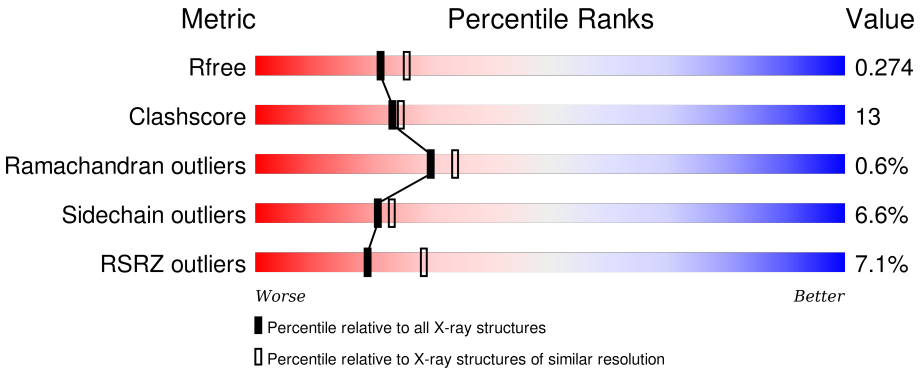
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.36 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}	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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. 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	242	13% 50% 28% • 19%
1	C	242	% 64% 15% • 18%
2	B	266	2% 66% 22% • 11%
2	D	266	8% 62% 27% • 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7094 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
1	A	196	Total	C	N	O	S	0	0	0
			1529	977	268	274	10			
1	C	198	Total	C	N	O	S	0	0	0
			1539	983	270	276	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	MET	-	EXPRESSION TAG	UNP P19793
A	222	LYS	-	EXPRESSION TAG	UNP P19793
A	223	LYS	-	EXPRESSION TAG	UNP P19793
A	224	GLY	-	EXPRESSION TAG	UNP P19793
C	221	MET	-	EXPRESSION TAG	UNP P19793
C	222	LYS	-	EXPRESSION TAG	UNP P19793
C	223	LYS	-	EXPRESSION TAG	UNP P19793
C	224	GLY	-	EXPRESSION TAG	UNP P19793

- Molecule 2 is a protein called Oxysterols receptor LXR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total	C	N	O	S	0	0	0
			1936	1235	339	355	7			
2	D	242	Total	C	N	O	S	0	0	0
			1964	1253	343	361	7			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	180	MET	-	EXPRESSION TAG	UNP Q9Z0Y9
B	181	ARG	-	EXPRESSION TAG	UNP Q9Z0Y9
B	182	GLY	-	EXPRESSION TAG	UNP Q9Z0Y9
B	183	SER	-	EXPRESSION TAG	UNP Q9Z0Y9

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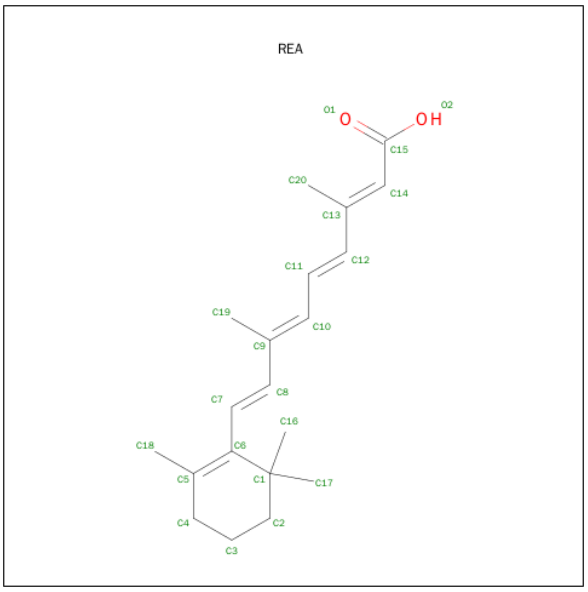
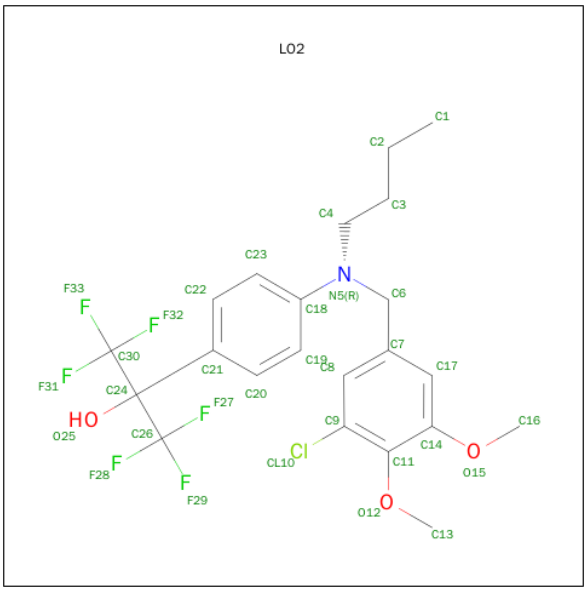
Chain	Residue	Modelled	Actual	Comment	Reference
B	184	HIS	-	EXPRESSION TAG	UNP Q9Z0Y9
B	185	HIS	-	EXPRESSION TAG	UNP Q9Z0Y9
B	186	HIS	-	EXPRESSION TAG	UNP Q9Z0Y9
B	187	HIS	-	EXPRESSION TAG	UNP Q9Z0Y9
B	188	HIS	-	EXPRESSION TAG	UNP Q9Z0Y9
B	189	HIS	-	EXPRESSION TAG	UNP Q9Z0Y9
B	190	GLY	-	EXPRESSION TAG	UNP Q9Z0Y9
B	191	MET	-	EXPRESSION TAG	UNP Q9Z0Y9
B	192	ALA	-	EXPRESSION TAG	UNP Q9Z0Y9
B	193	SER	-	EXPRESSION TAG	UNP Q9Z0Y9
B	194	LEU	-	EXPRESSION TAG	UNP Q9Z0Y9
B	195	VAL	-	EXPRESSION TAG	UNP Q9Z0Y9
B	196	PRO	-	EXPRESSION TAG	UNP Q9Z0Y9
B	197	ARG	-	EXPRESSION TAG	UNP Q9Z0Y9
B	198	GLY	-	EXPRESSION TAG	UNP Q9Z0Y9
B	199	SER	-	EXPRESSION TAG	UNP Q9Z0Y9
B	399	PRO	ARG	SEE REMARK 999	UNP Q9Z0Y9
D	180	MET	-	EXPRESSION TAG	UNP Q9Z0Y9
D	181	ARG	-	EXPRESSION TAG	UNP Q9Z0Y9
D	182	GLY	-	EXPRESSION TAG	UNP Q9Z0Y9
D	183	SER	-	EXPRESSION TAG	UNP Q9Z0Y9
D	184	HIS	-	EXPRESSION TAG	UNP Q9Z0Y9
D	185	HIS	-	EXPRESSION TAG	UNP Q9Z0Y9
D	186	HIS	-	EXPRESSION TAG	UNP Q9Z0Y9
D	187	HIS	-	EXPRESSION TAG	UNP Q9Z0Y9
D	188	HIS	-	EXPRESSION TAG	UNP Q9Z0Y9
D	189	HIS	-	EXPRESSION TAG	UNP Q9Z0Y9
D	190	GLY	-	EXPRESSION TAG	UNP Q9Z0Y9
D	191	MET	-	EXPRESSION TAG	UNP Q9Z0Y9
D	192	ALA	-	EXPRESSION TAG	UNP Q9Z0Y9
D	193	SER	-	EXPRESSION TAG	UNP Q9Z0Y9
D	194	LEU	-	EXPRESSION TAG	UNP Q9Z0Y9
D	195	VAL	-	EXPRESSION TAG	UNP Q9Z0Y9
D	196	PRO	-	EXPRESSION TAG	UNP Q9Z0Y9
D	197	ARG	-	EXPRESSION TAG	UNP Q9Z0Y9
D	198	GLY	-	EXPRESSION TAG	UNP Q9Z0Y9
D	199	SER	-	EXPRESSION TAG	UNP Q9Z0Y9
D	399	PRO	ARG	SEE REMARK 999	UNP Q9Z0Y9

- Molecule 3 is RETINOIC ACID (three-letter code: REA) (formula: $C_{20}H_{28}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 22 20 2	0	0
3	C	1	Total C O 22 20 2	0	0

- Molecule 4 is 2-{4-[BUTYL(3-CHLORO-4,5-DIMETHOXYBENZYL)AMINO]PHENYL}-1,1,1,3,3,3-HEXAFLUOROPROPAN-2-OL (three-letter code: LO2) (formula: $C_{22}H_{24}ClF_6NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C Cl F N O 33 22 1 6 1 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	D	1	Total	C	Cl	F	N	O	0	0
			33	22	1	6	1	3		

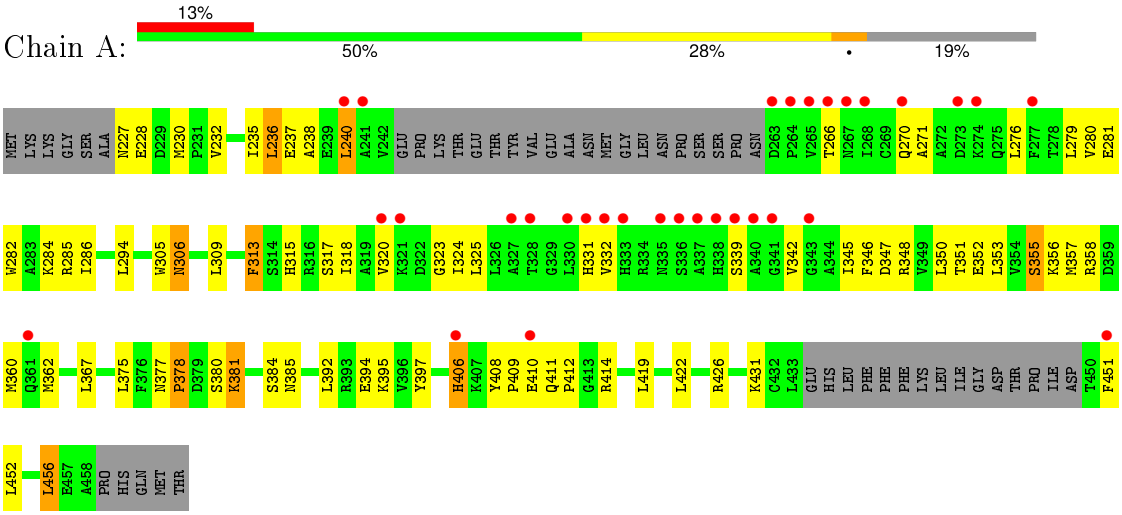
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	5	Total	O	0	0
			5	5		
5	C	4	Total	O	0	0
			4	4		
5	D	7	Total	O	0	0
			7	7		

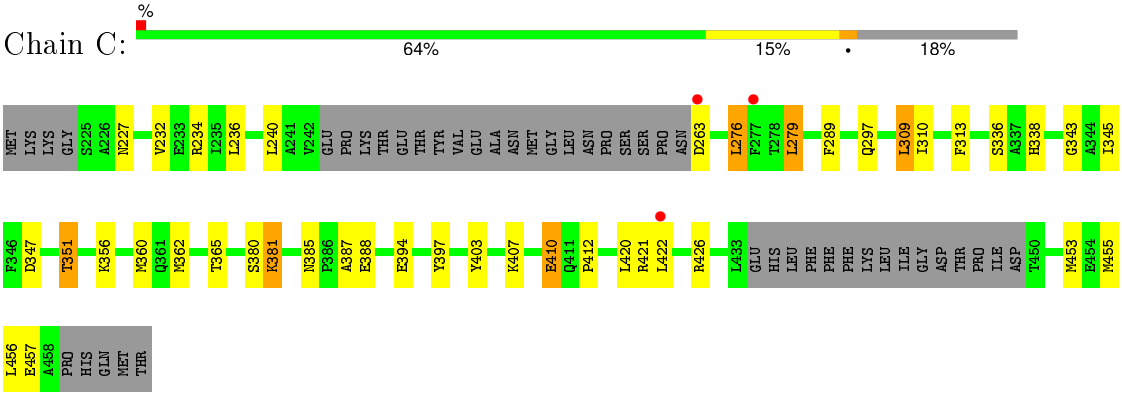
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

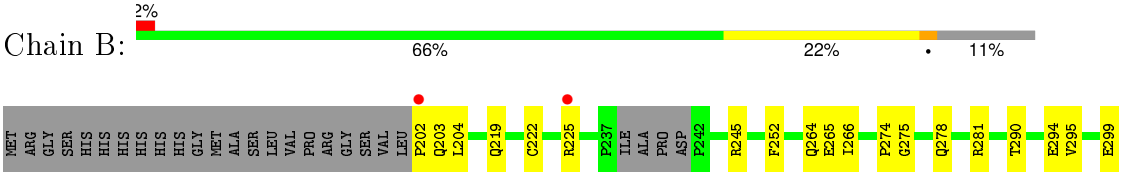
- Molecule 1: Retinoic acid receptor RXR-alpha

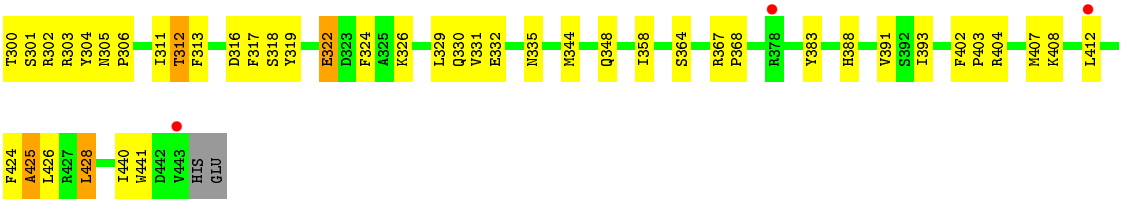


- Molecule 1: Retinoic acid receptor RXR-alpha

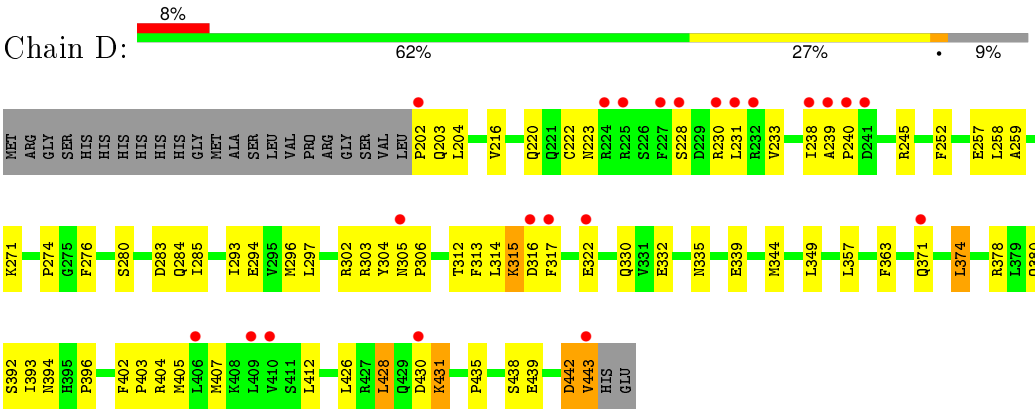


- Molecule 2: Oxysterols receptor LXR-alpha





- Molecule 2: Oxysterols receptor LXR-alpha



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	123.21Å 90.00Å 101.31Å 90.00° 111.88° 90.00°	Depositor
Resolution (Å)	42.34 – 2.36 42.34 – 2.36	Depositor EDS
% Data completeness (in resolution range)	98.5 (42.34-2.36) 98.5 (42.34-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.18 (at 2.37Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.219 , 0.278 0.220 , 0.274	Depositor DCC
R_{free} test set	2106 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.713	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 41749 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7094	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.44% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LO2, REA

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	0.34	0/1555	0.51	0/2100
1	C	0.42	0/1565	0.58	0/2114
2	B	0.47	0/1976	0.57	1/2673 (0.0%)
2	D	0.52	0/2006	0.56	1/2718 (0.0%)
All	All	0.45	0/7102	0.56	2/9605 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	202	PRO	N-CA-CB	7.24	111.99	103.30
2	D	202	PRO	N-CA-CB	7.02	111.72	103.30

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	1529	0	1565	56	0
1	C	1539	0	1572	30	0
2	B	1936	0	1939	47	0
2	D	1964	0	1966	63	0
3	A	22	0	27	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	22	0	27	3	0
4	B	33	0	24	4	0
4	D	33	0	24	5	0
5	B	5	0	0	0	0
5	C	4	0	0	0	0
5	D	7	0	0	0	0
All	All	7094	0	7144	190	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 13.

All (190) 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)
3:A:501:REA:H201	3:A:501:REA:O2	1.67	0.92
2:D:203:GLN:HA	2:D:393:ILE:HD11	1.52	0.88
4:B:1:LO2:H13A	4:B:1:LO2:O15	1.72	0.88
3:C:501:REA:O2	3:C:501:REA:H201	1.73	0.86
1:C:227:ASN:HD21	1:C:232:VAL:HB	1.39	0.84
2:D:391:VAL:HG21	2:D:405:MET:HE1	1.60	0.80
2:B:264:GLN:HA	1:C:455:MET:HE1	1.65	0.78
2:B:391:VAL:HG21	2:B:402:PHE:HB2	1.66	0.78
2:D:391:VAL:HG21	2:D:405:MET:CE	2.13	0.78
1:A:348:ARG:HG2	1:A:352:GLU:OE2	1.88	0.74
2:D:233:VAL:HG21	2:D:258:LEU:HD23	1.71	0.71
2:D:391:VAL:CG2	2:D:405:MET:HE1	2.21	0.71
4:B:1:LO2:H8	4:B:1:LO2:C18	2.21	0.70
2:B:290:THR:HG21	2:B:368:PRO:HD2	1.73	0.70
1:A:318:ILE:HG23	1:A:358:ARG:HG3	1.73	0.70
3:A:501:REA:C8	3:A:501:REA:H181	2.21	0.69
1:A:419:LEU:HD13	2:B:407:MET:HE1	1.72	0.69
1:A:353:LEU:O	1:A:357:MET:HG3	1.93	0.68
1:A:227:ASN:CG	1:A:228:GLU:H	1.97	0.68
2:B:440:ILE:HG22	2:B:441:TRP:CD1	2.30	0.67
2:D:252:PHE:CE1	2:D:431:LYS:HB3	2.31	0.66
1:A:381:LYS:N	1:A:381:LYS:HD2	2.12	0.65
2:B:364:SER:O	2:B:367:ARG:HG2	1.97	0.65
2:B:300:THR:HG23	2:B:311:ILE:HD13	1.78	0.65
2:D:252:PHE:CE2	2:D:426:LEU:HD13	2.32	0.65
3:C:501:REA:C8	3:C:501:REA:H181	2.27	0.64
2:B:264:GLN:HA	1:C:455:MET:CE	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ASN:ND2	1:C:232:VAL:HB	2.12	0.63
2:B:222:CYS:HB3	2:B:265:GLU:HG2	1.81	0.62
2:D:335:ASN:O	2:D:339:GLU:HG3	2.00	0.62
2:D:426:LEU:HD22	2:D:431:LYS:HG3	1.80	0.61
1:A:419:LEU:HD13	2:B:407:MET:CE	2.31	0.61
2:B:275:GLY:HA2	2:B:278:GLN:HG2	1.82	0.61
1:A:381:LYS:HD2	1:A:381:LYS:H	1.66	0.61
1:A:347:ASP:O	1:A:351:THR:HG23	2.01	0.60
4:D:1:LO2:C18	4:D:1:LO2:H8	2.32	0.60
2:D:322:GLU:CD	2:D:322:GLU:H	2.05	0.60
2:D:442:ASP:O	2:D:443:VAL:HG13	2.02	0.59
2:D:230:ARG:HG3	2:D:231:LEU:N	2.17	0.59
2:D:280:SER:O	2:D:284:GLN:HG3	2.02	0.59
1:A:456:LEU:O	2:D:271:LYS:HE2	2.03	0.59
1:A:394:GLU:OE2	2:B:404:ARG:HD3	2.01	0.59
1:C:227:ASN:HD21	1:C:232:VAL:H	1.51	0.58
2:D:303:ARG:HD3	2:D:312:THR:O	2.03	0.58
2:D:296:MET:HB3	4:D:1:LO2:C17	2.34	0.58
1:A:356:LYS:O	1:A:360:MET:HG2	2.04	0.58
2:B:204:LEU:HG	2:B:393:ILE:HD12	1.85	0.58
2:D:426:LEU:HB3	2:D:431:LYS:HB2	1.85	0.58
2:D:438:SER:O	2:D:442:ASP:HB2	2.04	0.58
2:D:374:LEU:O	2:D:378:ARG:HG3	2.04	0.57
1:A:410:GLU:O	1:A:412:PRO:HD3	2.04	0.57
2:D:314:LEU:O	2:D:317:PHE:HB2	2.04	0.57
1:C:410:GLU:H	1:C:410:GLU:CD	2.05	0.57
2:B:344:MET:SD	2:B:408:LYS:HG3	2.44	0.56
1:A:228:GLU:O	1:A:228:GLU:HG2	2.04	0.56
4:B:1:LO2:C13	4:B:1:LO2:O15	2.49	0.56
1:C:410:GLU:O	1:C:412:PRO:HD3	2.04	0.56
2:B:402:PHE:HB3	2:B:403:PRO:HD3	1.87	0.56
1:A:282:TRP:CZ3	1:A:375:LEU:HD22	2.42	0.55
4:D:1:LO2:H16B	4:D:1:LO2:H13A	1.88	0.55
1:A:348:ARG:NH2	1:A:431:LYS:HE3	2.21	0.54
2:D:203:GLN:CA	2:D:393:ILE:HD11	2.31	0.54
1:A:451:PHE:CZ	2:D:435:PRO:HB2	2.43	0.54
1:A:381:LYS:CD	1:A:381:LYS:H	2.19	0.54
2:D:238:ILE:O	2:D:238:ILE:HG22	2.07	0.54
1:A:280:VAL:O	1:A:284:LYS:HB2	2.08	0.54
2:D:283:ASP:OD2	2:D:371:GLN:HG2	2.07	0.54
2:B:300:THR:CG2	2:B:311:ILE:HD13	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:ASN:OD1	1:C:388:GLU:HB2	2.08	0.53
2:B:219:GLN:HE22	2:B:358:ILE:HD13	1.73	0.53
2:D:344:MET:HE1	2:D:349:LEU:HD12	1.91	0.53
2:B:281:ARG:HH21	1:C:457:GLU:HA	1.73	0.53
2:B:266:ILE:HG12	2:B:295:VAL:HG11	1.90	0.53
1:C:356:LYS:O	1:C:360:MET:HG2	2.09	0.53
1:C:347:ASP:O	1:C:351:THR:HG23	2.08	0.52
2:B:299:GLU:OE1	2:B:303:ARG:NH1	2.41	0.52
2:B:294:GLU:HG2	2:B:412:LEU:HB3	1.90	0.52
2:B:245:ARG:NH2	1:C:297:GLN:OE1	2.42	0.52
2:B:219:GLN:HE22	2:B:358:ILE:CD1	2.23	0.52
1:A:406:HIS:O	1:A:409:PRO:HD3	2.08	0.52
1:A:452:LEU:HD23	2:D:285:ILE:HG23	1.91	0.52
1:A:306:ASN:H	1:A:306:ASN:ND2	2.08	0.51
1:A:294:LEU:HD21	2:D:245:ARG:HG2	1.92	0.51
2:B:322:GLU:O	2:B:326:LYS:HG3	2.11	0.51
1:C:279:LEU:HD11	1:C:309:LEU:HD13	1.93	0.51
2:B:424:PHE:O	2:B:424:PHE:HD1	1.94	0.51
2:D:330:GLN:HB2	2:D:332:GLU:OE1	2.10	0.51
2:B:330:GLN:HB2	2:B:332:GLU:OE1	2.11	0.51
1:A:313:PHE:HE1	1:A:324:ILE:HG21	1.76	0.51
2:D:314:LEU:O	2:D:315:LYS:C	2.49	0.50
2:B:424:PHE:CD1	2:B:424:PHE:O	2.64	0.50
2:D:252:PHE:CZ	2:D:431:LYS:HB3	2.46	0.50
2:B:425:ALA:HA	2:B:428:LEU:HD22	1.93	0.50
1:C:338:HIS:ND1	1:C:343:GLY:HA3	2.27	0.50
2:B:203:GLN:HA	2:B:393:ILE:HD11	1.93	0.49
2:D:313:PHE:CE1	4:D:1:LO2:H16B	2.47	0.49
2:D:402:PHE:HB3	2:D:403:PRO:HD3	1.94	0.48
2:B:348:GLN:HA	2:B:348:GLN:HE21	1.78	0.48
1:C:407:LYS:HE2	1:C:407:LYS:HB2	1.63	0.48
1:C:381:LYS:H	1:C:381:LYS:HG2	1.44	0.48
2:B:302:ARG:HG3	2:B:302:ARG:O	2.12	0.48
2:D:294:GLU:HB3	2:D:412:LEU:HD13	1.96	0.47
1:A:451:PHE:HD2	2:D:439:GLU:OE2	1.97	0.47
2:B:324:PHE:HB3	2:B:329:LEU:HD12	1.95	0.47
2:D:304:TYR:CE1	2:D:306:PRO:HA	2.49	0.47
1:A:317:SER:HB3	1:A:324:ILE:HA	1.96	0.47
2:B:304:TYR:CE1	2:B:306:PRO:HA	2.49	0.47
2:D:322:GLU:N	2:D:322:GLU:CD	2.67	0.47
2:D:233:VAL:HG22	2:D:257:GLU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:GLY:HA3	1:A:332:VAL:O	2.15	0.47
1:A:236:LEU:O	1:A:240:LEU:HD13	2.15	0.47
1:C:455:MET:HE2	1:C:455:MET:HB3	1.80	0.47
1:A:350:LEU:O	1:A:355:SER:HB2	2.15	0.47
1:C:227:ASN:ND2	1:C:232:VAL:H	2.11	0.46
2:B:424:PHE:O	2:B:425:ALA:HB2	2.15	0.46
1:A:342:VAL:O	1:A:346:PHE:HB2	2.15	0.46
1:A:377:ASN:HA	1:A:378:PRO:HD3	1.79	0.46
2:D:315:LYS:O	2:D:316:ASP:HB2	2.16	0.46
2:D:231:LEU:C	2:D:233:VAL:H	2.18	0.46
2:B:317:PHE:HB3	2:B:319:TYR:CE2	2.50	0.46
1:C:394:GLU:OE2	2:D:404:ARG:HD3	2.17	0.45
2:B:312:THR:HB	2:B:318:SER:OG	2.16	0.45
3:A:501:REA:C8	3:A:501:REA:C18	2.91	0.45
3:C:501:REA:O2	3:C:501:REA:C20	2.52	0.45
1:A:227:ASN:CG	1:A:228:GLU:N	2.67	0.45
2:D:216:VAL:O	2:D:220:GLN:HG3	2.15	0.45
2:D:204:LEU:HG	2:D:393:ILE:HD12	1.98	0.45
2:D:276:PHE:CE2	2:D:284:GLN:HB3	2.51	0.45
2:D:222:CYS:HB3	2:D:265:GLU:HG3	1.98	0.45
1:C:232:VAL:HG13	1:C:365:THR:HG21	1.98	0.45
2:D:296:MET:HB3	4:D:1:LO2:H17	1.98	0.45
2:B:301:SER:HB2	2:B:344:MET:HB2	1.99	0.45
1:A:313:PHE:CE1	1:A:324:ILE:HG21	2.51	0.44
1:C:338:HIS:CE1	1:C:343:GLY:HA3	2.52	0.44
2:B:281:ARG:HG2	1:C:453:MET:HE1	1.99	0.44
2:D:274:PRO:HD2	2:D:383:TYR:OH	2.17	0.44
2:D:314:LEU:O	2:D:315:LYS:O	2.36	0.44
2:B:305:ASN:OD1	2:B:312:THR:HG22	2.17	0.44
1:A:236:LEU:O	1:A:236:LEU:HD22	2.17	0.44
1:C:279:LEU:HD11	1:C:309:LEU:CD1	2.48	0.44
1:C:310:ILE:HA	1:C:313:PHE:CE2	2.53	0.44
2:B:274:PRO:HD2	2:B:383:TYR:OH	2.18	0.44
1:A:392:LEU:HD23	1:A:395:LYS:HD2	2.00	0.44
1:A:236:LEU:HD22	1:A:240:LEU:HD13	2.00	0.43
1:C:397:TYR:OH	2:D:407:MET:HG2	2.17	0.43
2:B:313:PHE:CD1	4:B:1:LO2:H13B	2.52	0.43
2:D:239:ALA:HA	2:D:240:PRO:HD3	1.79	0.43
2:D:332:GLU:H	2:D:332:GLU:CD	2.20	0.43
1:A:271:ALA:HB3	3:A:501:REA:H203	1.99	0.43
1:C:385:ASN:HD21	1:C:387:ALA:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:281:ARG:HG2	1:C:453:MET:CE	2.48	0.43
1:A:306:ASN:HD22	1:A:306:ASN:H	1.66	0.43
1:A:315:HIS:CG	1:A:367:LEU:HD22	2.53	0.43
2:D:259:ALA:O	2:D:263:VAL:HG23	2.19	0.43
2:D:430:ASP:OD1	2:D:431:LYS:HD3	2.18	0.43
1:A:230:MET:CE	1:A:235:ILE:HD11	2.49	0.43
1:A:266:THR:HG22	1:A:270:GLN:OE1	2.19	0.43
2:D:293:ILE:O	2:D:297:LEU:HG	2.19	0.42
1:A:276:LEU:HA	1:A:276:LEU:HD23	1.71	0.42
1:A:362:MET:HA	1:A:414:ARG:NH2	2.34	0.42
2:D:231:LEU:C	2:D:233:VAL:N	2.73	0.42
2:D:391:VAL:HG11	2:D:402:PHE:HB2	2.02	0.42
1:C:276:LEU:HA	1:C:276:LEU:HD12	1.85	0.42
1:A:305:TRP:CD1	2:D:428:LEU:HD21	2.55	0.42
2:B:332:GLU:H	2:B:332:GLU:CD	2.23	0.42
1:A:279:LEU:HA	1:A:279:LEU:HD23	1.91	0.42
2:D:363:PHE:O	2:D:380:GLN:HB2	2.20	0.42
1:A:238:ALA:HB2	1:A:285:ARG:HB2	2.02	0.41
1:A:325:LEU:HD13	1:A:331:HIS:CE1	2.55	0.41
2:D:357:LEU:HA	2:D:357:LEU:HD12	1.87	0.41
1:A:394:GLU:HA	1:A:397:TYR:CD2	2.55	0.41
1:A:422:LEU:HA	1:A:422:LEU:HD23	1.91	0.41
1:A:356:LYS:HD3	1:A:356:LYS:HA	1.90	0.41
1:A:230:MET:HE1	1:A:286:ILE:HG23	2.03	0.41
2:B:252:PHE:CE2	2:B:426:LEU:HD13	2.55	0.41
2:D:230:ARG:HG3	2:D:231:LEU:H	1.84	0.41
1:A:408:TYR:N	1:A:409:PRO:CD	2.83	0.41
2:B:305:ASN:HA	2:B:306:PRO:HD2	1.92	0.41
1:A:411:GLN:OE1	1:A:414:ARG:HD2	2.20	0.41
1:C:289:PHE:CZ	1:C:297:GLN:HB3	2.56	0.41
2:D:305:ASN:HA	2:D:306:PRO:HD2	1.94	0.41
2:D:394:ASN:C	2:D:396:PRO:HD3	2.41	0.41
1:A:313:PHE:C	1:A:313:PHE:CD1	2.94	0.41
1:C:403:TYR:CE2	1:C:407:LYS:HE3	2.56	0.41
1:A:237:GLU:O	1:A:240:LEU:HB2	2.22	0.40
2:B:331:VAL:HG22	2:B:335:ASN:ND2	2.36	0.40
2:B:275:GLY:CA	2:B:278:GLN:HG2	2.49	0.40
1:A:317:SER:CB	1:A:324:ILE:HA	2.51	0.40
2:D:431:LYS:HG2	2:D:431:LYS:H	1.51	0.40
2:D:314:LEU:H	2:D:317:PHE:HB2	1.87	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	190/242 (78%)	176 (93%)	14 (7%)	0	100 100
1	C	192/242 (79%)	186 (97%)	6 (3%)	0	100 100
2	B	234/266 (88%)	226 (97%)	7 (3%)	1 (0%)	39 46
2	D	240/266 (90%)	228 (95%)	8 (3%)	4 (2%)	11 9
All	All	856/1016 (84%)	816 (95%)	35 (4%)	5 (1%)	30 34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	425	ALA
2	D	315	LYS
2	D	431	LYS
2	D	228	SER
2	D	442	ASP

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	164/208 (79%)	145 (88%)	19 (12%)	7 6
1	C	164/208 (79%)	145 (88%)	19 (12%)	7 6
2	B	215/239 (90%)	209 (97%)	6 (3%)	51 65
2	D	218/239 (91%)	212 (97%)	6 (3%)	51 65
All	All	761/894 (85%)	711 (93%)	50 (7%)	21 23

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	232	VAL
1	A	236	LEU
1	A	240	LEU
1	A	281	GLU
1	A	306	ASN
1	A	309	LEU
1	A	313	PHE
1	A	320	VAL
1	A	339	SER
1	A	345	ILE
1	A	355	SER
1	A	378	PRO
1	A	380	SER
1	A	381	LYS
1	A	384	SER
1	A	385	ASN
1	A	406	HIS
1	A	426	ARG
1	A	456	LEU
2	B	225	ARG
2	B	312	THR
2	B	316	ASP
2	B	322	GLU
2	B	388	HIS
2	B	428	LEU
1	C	234	ARG
1	C	236	LEU
1	C	240	LEU
1	C	263	ASP
1	C	276	LEU
1	C	279	LEU
1	C	309	LEU
1	C	336	SER
1	C	345	ILE
1	C	351	THR
1	C	362	MET
1	C	380	SER
1	C	381	LYS
1	C	410	GLU
1	C	420	LEU
1	C	421	ARG
1	C	422	LEU

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Mol	Chain	Res	Type
1	C	426	ARG
1	C	456	LEU
2	D	223	ASN
2	D	302	ARG
2	D	374	LEU
2	D	392	SER
2	D	428	LEU
2	D	443	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	306	ASN
1	A	331	HIS
1	A	385	ASN
2	B	348	GLN
1	C	227	ASN
1	C	335	ASN
1	C	385	ASN
2	D	335	ASN

5.3.3 RNA

There are no RNA molecules 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

4 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	REA	A	501	-	19,22,22	1.15	1 (5%)	26,30,30	1.65	6 (23%)
4	LO2	B	1	-	34,34,34	0.84	0	50,51,51	1.45	4 (8%)
3	REA	C	501	-	19,22,22	1.11	1 (5%)	26,30,30	1.58	5 (19%)
4	LO2	D	1	-	34,34,34	0.86	1 (2%)	50,51,51	1.56	4 (8%)

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	REA	A	501	-	-	0/13/32/32	0/1/1/1
4	LO2	B	1	-	-	0/40/40/40	0/2/2/2
3	REA	C	501	-	-	0/13/32/32	0/1/1/1
4	LO2	D	1	-	-	0/40/40/40	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	REA	C1-C6	-3.26	1.49	1.53
3	C	501	REA	C1-C6	-3.00	1.49	1.53
4	D	1	LO2	C24-C21	-2.07	1.50	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1	LO2	C16-O15-C14	-8.08	105.28	117.54
4	B	1	LO2	C16-O15-C14	-6.34	107.93	117.54
3	C	501	REA	C7-C8-C9	-4.46	119.41	126.22
4	D	1	LO2	C4-N5-C18	-3.81	115.36	121.10
3	A	501	REA	C18-C5-C6	-3.62	121.05	124.61
3	A	501	REA	C7-C8-C9	-3.34	121.13	126.22
3	A	501	REA	C3-C4-C5	-3.25	108.70	113.87
4	B	1	LO2	C13-O12-C11	-3.23	106.34	114.82
3	C	501	REA	C18-C5-C6	-3.19	121.47	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	501	REA	C3-C4-C5	-2.91	109.25	113.87
4	B	1	LO2	C4-N5-C18	-2.69	117.03	121.10
4	B	1	LO2	C9-C8-C7	-2.53	118.73	120.36
3	A	501	REA	C19-C9-C10	-2.26	119.56	122.90
4	D	1	LO2	C13-O12-C11	-2.23	108.96	114.82
3	C	501	REA	C3-C2-C1	-2.08	107.13	114.83
3	A	501	REA	C10-C11-C12	-2.03	116.94	123.13
4	D	1	LO2	C11-C9-CL10	2.58	121.59	118.43
3	C	501	REA	C8-C9-C10	2.59	123.16	118.98
3	A	501	REA	C8-C9-C10	3.46	124.55	118.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	REA	4	0
4	B	1	LO2	4	0
3	C	501	REA	3	0
4	D	1	LO2	5	0

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	196/242 (80%)	1.00	32 (16%) 2 4	26, 51, 66, 80	0
1	C	198/242 (81%)	0.38	3 (1%) 76 85	18, 30, 47, 58	0
2	B	238/266 (89%)	0.38	5 (2%) 67 79	20, 32, 52, 71	0
2	D	242/266 (90%)	0.66	22 (9%) 11 18	20, 34, 69, 91	0
All	All	874/1016 (86%)	0.60	62 (7%) 19 28	18, 35, 62, 91	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	202	PRO	7.4
2	D	238	ILE	6.5
2	D	443	VAL	6.2
2	D	231	LEU	6.2
2	D	230	ARG	6.0
2	D	240	PRO	5.9
2	D	228	SER	5.4
2	B	443	VAL	5.1
1	A	264	PRO	4.8
1	A	263	ASP	4.7
2	B	202	PRO	4.2
1	A	274	LYS	4.1
1	A	339	SER	4.1
2	D	316	ASP	3.8
1	A	340	ALA	3.8
1	A	335	ASN	3.6
1	A	320	VAL	3.6
1	A	241	ALA	3.5
1	A	327	ALA	3.5
1	A	410	GLU	3.5
1	A	336	SER	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	317	PHE	3.3
1	A	277	PHE	3.3
1	A	273	ASP	3.3
1	A	266	THR	3.3
2	D	232	ARG	3.3
1	A	270	GLN	3.2
2	D	430	ASP	3.2
1	A	330	LEU	3.2
1	A	338	HIS	3.1
1	A	328	THR	3.1
2	D	239	ALA	3.1
1	A	240	LEU	3.1
2	D	227	PHE	3.1
1	C	422	LEU	3.0
1	A	406	HIS	3.0
1	A	333	HIS	3.0
2	B	412	LEU	3.0
2	B	378	ARG	2.8
1	A	337	ALA	2.7
2	D	322	GLU	2.6
1	A	343	GLY	2.6
2	D	225	ARG	2.6
2	D	305	ASN	2.6
1	A	331	HIS	2.6
1	C	263	ASP	2.5
1	A	361	GLN	2.5
1	A	265	VAL	2.4
1	A	332	VAL	2.3
2	D	409	LEU	2.3
2	B	225	ARG	2.3
1	A	341	GLY	2.3
1	A	321	LYS	2.2
2	D	410	VAL	2.2
2	D	224	ARG	2.2
1	A	268	ILE	2.2
2	D	241	ASP	2.2
1	A	451	PHE	2.1
1	A	267	ASN	2.1
1	C	277	PHE	2.1
2	D	371	GLN	2.0
2	D	406	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 carbohydrates in this entry.

6.4 Ligands (i)

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, 95^{th} 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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	REA	A	501	22/22	0.86	0.20	0.10	44,51,55,56	0
3	REA	C	501	22/22	0.94	0.14	-0.16	25,31,38,41	0
4	LO2	B	1	33/33	0.95	0.13	-0.49	21,27,35,45	0
4	LO2	D	1	33/33	0.96	0.13	-0.82	27,34,41,55	0

6.5 Other polymers (i)

There are no such residues in this entry.